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A GENERAL METHOD FOR CALCULATING
THE SPECIFIC IMPULSE OF
HIGH ENERGY PROPELLANT MIXTURES

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ABSTRACT

The method employed by The Dow Chemical Company for calculating specific impulses of propellant mixtures is described. Although the method is general, the capacity of the computer (Burroughs 220) and the availability of thermodynamic data place practical restrictions on what systems can be calculated. The calculations center around the method of White, Johnson, and Dantzig for determining the equilibrium compositions of complex mixtures. By developing and applying matrix equations which describe both the thermodynamic data and the physical equations, the programming effort has been reduced significantly. Required input data to the program are the composition of the reaction mixture, the chamber and exit pressures, and a rough estimate of the chamber temperature. All other pertinent data are retrieved from magnetic tape by the computer program. The program is automatic in that a large number of problems may be solved without manual intervention. In addition to the specific impulse, the program calculates the characteristic velocity, the chamber and exit temperatures, compositions, enthalpies and entropies.

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I. INTRODUCTION

The theoretical specific impulse of a propellant system has been used extensively as an indicator to evaluate the maximum performance which could be expected from the system. The calculation of the specific impulse allows rapid and relatively inexpensive screening of the many candidate systems. Earlier work, previously reported^{1,2}, at this Laboratory by R. R. V. Wiederkehr resulted in a general method programmed for a Burroughs 220 Computer.

Recently, the capabilities of the Dow Burroughs 220 were enlarged; therefore, expansion of the computational program was undertaken. The basic mathematical model remained unchanged, but the setup, input, and output sections were extensively revised.

Although the basic method has been discussed in the previously cited reports, for the sake of unity and clarity an exhaustive treatment of the theory and modus operandi of the program will be included in this report.

Specific impulse has been defined as the velocity of the products at the exhaust divided by the gravitational constant. If the change in enthalpy of the chamber products as they are expanded through a nozzle is equated to the kinetic energy of the particles, the specific impulse may be defined as:

$$I_{sp} = c \left[\frac{H_c - H_e}{\mu} \right]^{1/2} \quad (1)$$

where, H_c is the enthalpy of μ grams of products in the rocket chamber,

H_e is the enthalpy of μ grams of products in the nozzle exit, and

c is a constant.

In order to calculate the specific impulse one must merely determine values of H_c and H_e . Assuming no heat losses to the surroundings, a heat balance in which the enthalpy of the reactants is converted to the enthalpy of the products may be written:

$$\sum_{j=1}^p r_j \Delta H_{e_j} = H_c \quad (2)$$

where, r_j is the number of moles of the j th reactant in the reaction mixture,

ΔH_f_j is the heat of formation of the j th reactant at 298°K., and

p is the number of reactants.

To obtain H_e , the equilibrium composition at a chamber temperature must be determined such that equation (2) is satisfied and then an exhaust temperature and composition must be chosen such that there is an entropy balance, $S_c = S_e$, since isentropic flow has been assumed. From this exhaust composition the exit enthalpy, H_e , can be easily calculated as a function of temperature. All the necessary information for the calculation of the specific impulse by equation (1) is then available.

It is recognized that during expansion the reaction products undergo chemical change. The extent of this change cannot be ascertained by theoretical means. It has been assumed, therefore, that complete chemical equilibrium is maintained during the expansion process.

The overall problem may be considered as two separate and identical problems which are merely the determination of a chemical equilibrium composition at a given temperature. The temperatures desired are fixed by the enthalpy balance in the case of the chamber solution and by the entropy balance in the case of the exhaust solution as illustrated in Table I.

Table I

Relation of Temperature with Enthalpy and Entropy Balance

<u>Find T, X such that</u>	<u>Use T, X to Calculate</u>
Chamber: $H(T_c, X_c, P_c) = H_c$	S_c
Exhaust: $S(T_e, X_e, P_e) = S_c$	H_e and I_{sp}

A double trial and error scheme is used to find the desired temperature and composition in each of the two problems. Starting with an assumed temperature, the corresponding equilibrium composition is obtained by a trial and error procedure and then the left side of the equation in Table I is computed using this temperature and composition. If equality is obtained (within practical limits), the assumed temperature is the desired temperature and the composition is the desired composition. If equality is not obtained an improved temperature is assumed.

The magnitude of the improvement is dependent on the magnitude and direction of the inequality. The equilibrium temperature is again calculated and the process repeated until equality is attained.

It is evident that the solution to the problem revolves around a method for determining the compositions and temperatures. This report will consider the following:

- (i) Method for calculating composition (Section II).
- (ii) Method for calculating temperatures (Section III).
- (iii) Method for generating thermodynamic functions (Section IV).
- (iv) Description of the operation, input, output, and capabilities of the computer program.

II. CALCULATION OF THE EQUILIBRIUM COMPOSITION OF A MULTICOMPONENT SYSTEM*

From the first and second laws of thermodynamics it can be shown that a system at constant temperature and pressure achieves equilibrium when the free energy of the system is a minimum. Equilibrium is achieved when the composition is such that the free energy is minimized. This principle is used to calculate the equilibrium compositions of multicomponent systems.

The method used for minimizing the free energy of a system is essentially that of White, Johnson, and Dantzig³ as extended by Thomson⁴ to include condensed species*.

The method performs the following operation: given any composition $Y = (y_1, y_2, y_3 \dots y_n)$ compatible with the mass balance constraints, an improved composition $X = (x_1, x_2, x_3 \dots x_n)$ is calculated which is closer to the equilibrium value. If X is not sufficiently close to the equilibrium value, it becomes the new Y , which can be improved further. The procedure is repeated until convergence is achieved.

*This section is taken almost in its entirety from Report Nr. AR-1S-60, by R. R. V. Wiederkehr (Reference (1)).

A. Composition Convergence Method

The free energy of the system with a composition of X is*:

$$F_r(X) = \sum_{i=1}^{n_g} \left[\left(\frac{F_i}{RT} \right) + \ln P + \ln \frac{x_i}{\bar{x}} \right] x_i + \sum_{i=n_g+1}^{n_g+n_c} \frac{F_i}{RT} x_i \quad (3)$$

$$\text{where, } \bar{x} = \sum_{i=1}^{n_g} x_i. \quad (4)$$

The summation in (4) extends over only the gaseous components. The first summation on the right of (3) is the free energy of the gaseous species; the second term is the free energy of the condensed species. The entropy of mixing of the condensed phases is assumed negligible, and the gases are assumed to be ideal.

The behavior of the free energy in the neighborhood of Y may be approximated by a Taylor's expansion, about Y:

$$Q(X) = F_r(Y) + \sum_{i=1}^{n_g+n_c} \left. \frac{\partial F}{\partial x_i} \right|_{X=Y} (x_i - y_i) + \frac{1}{2} \sum_{i=1}^{n_g+n_c} \sum_{k=1}^{n_g+n_c} \left. \frac{\partial^2 F}{\partial x_i \partial x_k} \right|_{X=Y} (x_i - y_i)(x_k - y_k) \quad (5)$$

which reduces to:

$$Q(X) = F_r(X) + \sum_{i=1}^{n_g} \left[\left(\frac{F_i}{RT} \right) + \ln P + \ln \frac{y_i}{\bar{y}} \right] (x_i - y_i) + \sum_{i=n_g+1}^{n_g+n_c} \left(\frac{F_i}{RT} \right) (x_i - y_i) + \frac{1}{2} \sum_{i=1}^{n_g} y_i \left[\frac{(x_i - y_i)}{y_i} - \frac{(\bar{x} - \bar{y})}{\bar{y}} \right]^2 \quad (6)$$

* $F_r(X)$ is actually free energy divided by RT.

It is desired to minimize the quadratic approximation to the free energy $Q(X)$ subject to the element balance restraints given by:

$$\sum_{i=1}^{n_c+n_g} a_{ij}x_i = b_j \quad (7)$$

where a_{ij} are formula numbers indicating the number of atoms of element j in a molecule of species i , and b_j is the total number of atomic weights of element j originally present in the mixture; m is the number of elements in the system.

The constraints and $Q(X)$ may be incorporated into a single equation:

$$G(X) = Q(X) + \sum_{j=1}^m \pi_j \left(\sum_i a_{ij}x_i + b_j \right) \quad (8)$$

where the π_j 's are Lagrange multipliers.

To minimize $G(X)$, $\frac{\partial G}{\partial x_1}$ is set equal to zero. It can be shown via (6) and (8) that for the gaseous components:

$$\frac{\partial G}{\partial x_1} = \left[\left(\frac{F_1}{RT} \right) + \ln P_2 \ln \frac{y_1}{\bar{y}} \right] + \left[\frac{x_1}{y_1} - \frac{\bar{x}}{\bar{y}} \right] - \sum_{j=1}^m \pi_j a_{1j} = 0$$

$i=1, 2, \dots, n_g$ (9)

but for the condensed components:

$$\frac{\partial G}{\partial x_i} = \frac{F_i}{RT} - \sum_1^m \pi_j a_{ij} = 0 \quad i=n_g+1, n_g+2, \dots, n_g+n_c \quad (10)$$

There are n_g equations of type (9), n_c of type (10), m constraining equations (7), and equation (4). At this point, therefore, there are $n_g + m + 1$ equations and as many unknowns. But by

solving (9) for n_g of the x_i 's and substituting these x_i 's into equations (7) and (4), the number of unknowns is reduced to $n_c + m + 1$. Solving (9) for x_1 yields:

$$x_1 = -y_1 \mathcal{F}_1 + \left(\frac{y_1}{\bar{y}} \right) \bar{x} + \left(\sum_{j=1}^m \pi_j a_{1j} \right) \quad y_1 \quad i=1, 2, \dots, n_g \quad (11)$$

$$\text{where } \mathcal{F}_1 = \left[\left(\frac{F_1}{RT} \right) + \ln P + \ln \frac{y_1}{\bar{y}} \right] \quad (12)$$

Substitution of (11) into (4) and (7) produces:

$$\sum_{j=1}^m \left[\sum_{i=1}^{n_g} a_{ij} y_i \right] \pi_j = \sum_{i=1}^{n_g} y_i \mathcal{F}_i \quad (13)$$

$$\text{and } \sum_{k=1}^m \left[\sum_{i=1}^{n_g} a_{ij} a_{ik} y_i \right] \pi_k + \left[\sum_{i=1}^{n_g} a_{ij} y_i \right] \frac{\bar{x}}{\bar{y}} + \sum_{i=n_g+1}^{n_g+n_c} a_{ij} x_i = \\ b_j + \sum_{i=1}^{n_g} a_{ij} y_i \mathcal{F}_i \quad (14)$$

The problem of minimizing the free energy subject to mass balance constraints reduces to solving equations (14), (10), and (13) simultaneously.

It can be shown that these equations can be rewritten in matrix notation as follows:

$$(A'_g Y_{gd} A_g) \pi + A'_c X_c + A'_g Y_g \frac{\bar{x}}{\bar{y}} = B + A'_g Y_{gD} \mathcal{F}_g \quad (15)$$

$$A_c \pi = \mathcal{F}_c \quad (16)$$

$$Y'_g A_g \pi = Y'_g \mathcal{F}_g \quad (17)$$

where the matrices are defined as follows:

$$A_g = \begin{bmatrix} a_{11} & a_{12} & \dots & a_{1m} \\ a_{21} & & & \\ \vdots & & & \\ a_{ng,1} & \dots & \dots & a_{ng,m} \end{bmatrix}_{n_g \times m}$$

$$A_c = \begin{bmatrix} a_{ng+1,1} & \dots & a_{ng+1,m} \\ \vdots & & \\ a_{ng+n_c,1} & \dots & a_{ng+n_c,m} \end{bmatrix}_{n_c \times m}$$

$$\mathcal{J}_g = \begin{bmatrix} \frac{F_1}{RT} \\ \frac{F_2}{RT} \\ \vdots \\ \frac{F_{ng}}{RT} \end{bmatrix} \quad Y_g = \begin{bmatrix} y_1 \\ y_2 \\ \vdots \\ y_{ng} \end{bmatrix}$$

$$\mathcal{J}_c = \begin{bmatrix} \frac{F_{ng+1}}{RT} \\ \frac{F_{ng+2}}{RT} \\ \vdots \\ \frac{F_{ng+n_c}}{RT} \end{bmatrix} \quad Y_{GD} = \begin{bmatrix} y_1 & 0 & 0 & \dots & 0 \\ 0 & y_2 & 0 & & \\ 0 & 0 & y_3 & & \\ 0 & \dots & & \ddots & 0 \\ & & & & y_{ng} \end{bmatrix}$$

$$\pi = \begin{bmatrix} \pi_1 \\ \pi_2 \\ \vdots \\ \pi_m \end{bmatrix} \quad X_g = \begin{bmatrix} x_1 \\ x_2 \\ \vdots \\ x_{ng} \end{bmatrix}$$

$$B = \begin{bmatrix} b_1 \\ b_2 \\ \vdots \\ b_m \end{bmatrix} \quad X_c = \begin{bmatrix} x_{ng+1} \\ \vdots \\ x_{ng+n_c} \end{bmatrix}$$

The superscript ¹ designates the transposition of a matrix.

Equations (15), (16) and (17) may be combined to give a single matrix equation:

$$\begin{matrix} m \\ n_c \\ 1 \end{matrix} \left\{ \begin{bmatrix} A'g & Y_{gD} & A_g & | & A'_c & A_g'Y_g \\ \hline & & & | & & \\ & A_c & & | & 0 & 0 \\ \hline & Y'_g & A_g & | & 0 & 0 \end{bmatrix} \begin{bmatrix} \pi \\ X_c \\ \bar{x}/\bar{y} \end{bmatrix} \right. = \left. \begin{bmatrix} B + A'_g & Y_{gD} & \mathcal{J}_g \\ \hline & & \\ & \mathcal{J}_c & \\ \hline & Y'_g & \mathcal{J}_g \end{bmatrix} \right\} \quad (18)$$

This equation represents a system of $m + n_c + 1$ linear equations with as many unknowns. The brackets and symbols indicate the dimensions of the matrices.

The unknowns are: $\pi = (\pi_1, \pi_2, \dots, \pi_m)$,

$X_c = (x_{n_g+1}, x_{n_g+2}, \dots, x_{n_g+n_c})$, and

\bar{x}/\bar{y} .

Solving Equation (18) for the unknowns yields:

$$\begin{bmatrix} \pi \\ X_c \\ \bar{x}/\bar{y} \end{bmatrix} = \begin{bmatrix} A'g & Y_{gD} & A_g & | & A'_c & A_g'Y_g \\ \hline & & & | & & \\ & A_c & & | & 0 & 0 \\ \hline & Y'_g & A_g & | & 0 & 0 \end{bmatrix}^{-1} \begin{bmatrix} B + A'_g & Y_{gD} & \mathcal{J}_g \\ \hline & & \\ & \mathcal{J}_c & \\ \hline & Y'_g & \mathcal{J}_g \end{bmatrix} \quad (19)$$

The square matrix to be inverted may be calculated from Y and the formula numbers a_{ij} . The vector on the right may be calculated from Y , a_{ij} , and the \mathcal{J}_g and \mathcal{J}_c vectors. It will be shown in Section IV-A how the \mathcal{J}_g and \mathcal{J}_c vectors (partial free energy vectors) may be simply calculated. Therefore, given Y , the formula numbers, and the partial free energy vectors, one may calculate: the number of moles of each condensed species at equilibrium, X_c , the Lagrangian multipliers π , and \bar{x}/\bar{y} . The number of moles of each gaseous species at equilibrium may be calculated from Equation (11). In matrix notation Equation (11) is

$$X_g = Y_{gD} \left[\left(\frac{\bar{x}}{\bar{y}} \right) - \mathcal{J}_g + A_g \pi \right] \quad (20)$$

where both X_g and $\left[\left(\frac{\bar{x}}{\bar{y}} \right) - \mathcal{J}_g + A_g \pi \right]$ are $(n_g \times 1)$ vectors, and Y_{gD} is a $(n_g \times n_g)$ diagonal matrix. In (20) $\left(\frac{\bar{x}}{\bar{y}} \right)$ represents a $(n_g \times 1)$ column matrix whose elements are all $\frac{\bar{x}}{\bar{y}}$.

At a given temperature the thermal data and the formula numbers are fixed. Hence, Equations (19) and (20) provide a scheme for obtaining an improved estimate of the equilibrium composition, X , from an original estimate Y . The vector Y may be regarded as an input to our scheme which produces an output X . The resulting X becomes the new Y and the procedure is repeated until X and Y balance.

It is not practical to continue the procedure until an exact balance of X and Y is obtained, since this would take an inordinate amount of time. Therefore, the following criterion is used:

$$\text{If for all } y_i \quad [x_i - y_i]_{\max.} < 0.0005 \quad (21)$$

Then X is assumed to be in balance with Y .

B. Convergence Difficulties

Certain difficulties may arise during the process of balancing X and Y , i.e., calculated values of x_i may be negative, the square matrix in equation (9) may fail to invert, or X may continuously oscillate about Y and never quite converge. There follows a discussion of how each of these difficulties may be circumvented.

1. Negative Values of x_i

It sometimes happens that values of x_i calculated by the above method are negative. Physically this has no significance since the number of moles of any species x_i must be zero or positive. To rectify this condition when it occurs, the following procedure is followed:

$$\Delta = X - Y \quad (22)$$

which represents the recommended step needed to improve the compositions. If one or more of the x_i 's are negative the recommended step is too large. Therefore, it is reasonable to merely shorten this recommended step by a factor λ so as to make each of the x_i 's positive. The new values of x_i are given by:

$$X_{\text{new}} = Y + \lambda \Delta \quad (23)$$

for each x_i which is negative let a λ_i be calculated according to the equation.

$$\lambda_i = \frac{-y_i}{\Delta_i} \quad (24)$$

Substitution of this λ_i into Equation (23) causes x_i new to be zero. If a λ larger than λ_i were used, x_i new would remain negative. Therefore, of all the λ_i calculated, the smallest must be chosen. This value of λ , viz., λ_s , will cause x_s new to be zero, and all other x_i 's to be positive.

a. Gaseous Species - For gaseous species, zero is an objectionable value to use for x_s since, according to equation (20), this estimate can never be improved but will remain zero. Instead of letting x_s go to zero, the following scheme is used: Arbitrarily values are given to x_s depending on the size of the corresponding y_s , that is,

$$\text{if } y_s > 1 \times 10^{-11}, \quad x_s = 1 \times 10^{-11} \quad (25a)$$

or

$$\text{if } 1 \times 10^{-11} > y_s > 1 \times 10^{-31}, \quad x_s = 1 \times 10^{-31} \quad (25b)$$

or

$$\text{if } y_s < 1 \times 10^{-31}, \quad x_s = 0 \quad (25c)$$

If y_s is small enough, x_s does become zero. Since this would preclude the possibility of any further modification or improvement to this species, when convergence has been attained all zero values are arbitrarily set at a value of 1×10^{-6} and the iteration repeated until X and Y balance again. This device is a radical departure from the previously reported method¹ and has proved to be more efficient. Every time a new temperature is used the device,

$$\text{if } x_i = 0, y_i \text{ new} = 1 \times 10^{-6} \quad (26)$$

is also used.

b. Condensed Species - For condensed species a zero value for x_s is not objectionable. Consequently, using λ_s alone is sufficient.

Another difficulty may arise, however. If x_i for a condensed species is zero (which means y_i for the next iteration is also zero) and the following x_i is negative, an impasse is reached.

Clearly λ_i calculated from Equation (24) is zero so that $X_{\text{new}} = Y_{\text{old}}$ [see Equation (23)]. A λ of zero prevents X from improving.

III. CALCULATION OF THE CHAMBER AND EXIT TEMPERATURES

Two temperatures, the chamber temperature and the exhaust temperature, must be determined in the course of the solution of the problem. The desired temperature is obtained when the enthalpy of entropy of the system equals the chamber enthalpy or entropy respectively (See Table I). Since the methods used for the two temperatures are similar, only the case of the chamber temperature will be considered.

Starting with an assumed temperature, T , the enthalpy of the system is calculated and compared with the chamber enthalpy. If the calculated enthalpy is low (high), then the next temperature is increased (decreased). This new "improved temperature," T_{n+1} is calculated according to the following linear interpolation or extrapolation formula:

$$T_{n+1} = T_n + \phi_H (H_c - H_n) \quad (27)$$

where H_n is given by Equation (55) and H_c is given by Equation (2). To calculate the second temperature from the assumed first temperature a value for ϕ_H of $0.01 + K./cal.$ is used. For succeeding temperature ϕ_H is given by:

$$\phi_H = \frac{T_n - T_{n-1}}{H_n - H_{n-1}} \quad (28)$$

Equation (27) is used for extrapolation to new temperature until the chamber temperature has been straddled. Once the chamber temperature has been straddled, Equation (28) is used for interpolation.

Equation (27) has certain shortcomings. When the temperatures T_n and T_{n-1} straddle both the chamber temperature and a phase transition temperature, Equation (27) produces a very poor "improved temperature." This is a result of the very non-linear behavior of H with T in the neighborhood of a phase transition; the enthalpy abruptly changes across the transition (See Figure 1). When this difficulty arises it can be eliminated by the following method which is based on Figure 1.

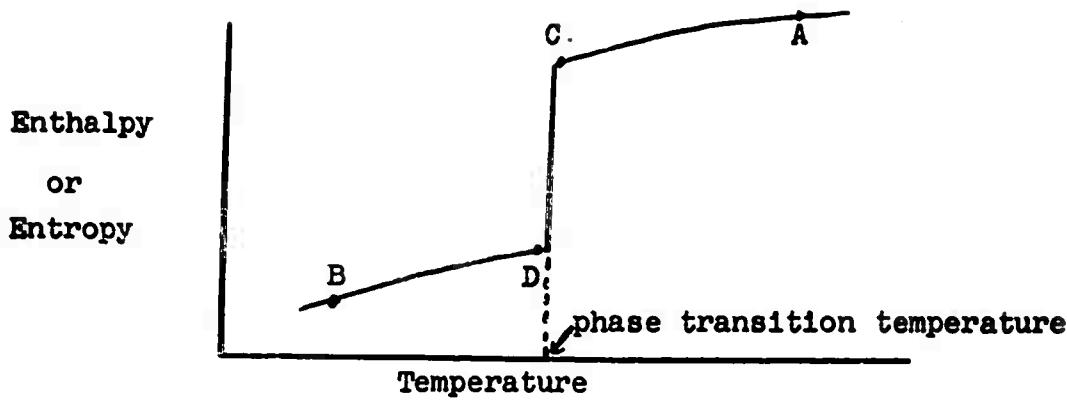


Fig. 1 - Schematic of Non-Linear Behavior
of Enthalpy with Temperature

Suppose that the two temperatures which straddle both the chamber temperature and a phase transition temperature yield the points A and B on Figure 1. By calculating the enthalpy of the system at a temperature slightly ($0.5^{\circ}\text{K}.$) above and below the phase transition temperature, the points C and D are obtained. If the chamber enthalpy is between the enthalpies of points A and C or B and D, Equation (27) is applied using the points A and C or B and D, respectively. However, if the chamber enthalpy lies between the enthalpies of points C and D, then the chamber temperature coincides with the phase transition temperature and the compound undergoing the phase transition must be partly in one phase and partly in the other.

In general, the composition of the system varies upon traversing a phase transition. The phase transition composition (chamber composition) may be calculated on the assumption that the composition varies linearly with the enthalpy across the transition. From the enthalpies and compositions corresponding to C and D and the chamber enthalpy, the chamber composition can be calculated.

To this point the discussion has been concerned with choosing improved temperatures. When an improved temperature T is obtained such that:

$$H(T, X) - H_C < 100 \text{ cal.} \quad (29)$$

then that temperature T is defined as the chamber temperature T_C . In the above equation $H(T, X)$ is given by (55) and H_C is given by (2). The convergence criterion for the exhaust solution is:

$$\text{If } S(T, X, P_e) - S_C < 0.02 \text{ e.u.} \quad (30)$$

then the temperature is the exit temperature. In this equation S_c is evaluated according to (65) using the chamber conditions and $S(T, X, P_e)$ is calculated by (65) at the assumed exit conditions.

IV. THE GENERATION OF THERMODYNAMIC PROPERTIES BY THE USE OF MATRICES

A. The Matrix Representation of the Enthalpy, Entropy, and Free Energy*

To calculate the chamber conditions it is necessary to be able to evaluate the enthalpy as a function of temperature, composition, and pressure. To calculate the exit conditions it is necessary to be able to evaluate the entropy as a function of temperature, composition, and pressure. To calculate the equilibrium composition it is necessary to know the partial free energies as a function of temperature, pressure, and composition. This section shows how these thermodynamic functions can be concisely represented and simply generated by the use of matrices.

1. Single Species System

The enthalpy of a single species (i.e., a compound in a given phase) at a given pressure as a function of temperature can be evaluated if the heat capacity as a function of temperature and the enthalpy at some base temperature, T_b , are known:

$$H(T) = H(T_b) + \int_{T_b}^T C_p(t) dt \quad (31)$$

The molar entropy of a species as a function of temperature at a given pressure can also be evaluated if the heat capacity as a function of temperature and the entropy at some base temperature, T_b , are known:

$$S(T) = S(T_b) + \int_{T_b}^T \frac{C_p(t)}{T} dt \quad (32)$$

The molar free energy of a compound can be evaluated according to the equation:

$$F(T) = H(T) - TS(T) \quad (33)$$

Therefore, given the heat capacity as a function of temperature, and the enthalpy and entropy at some base temperature, T_b , one can evaluate the enthalpy, entropy, and free energy as functions of temperature at a given pressure.

*This section is also taken in its entirety from R. R. V. Wiederkehr, Report No. AR-1s-60.

Maier and Kelly* have successfully described the heat capacity as a function of temperature using the equation:

$$C_p = a + bT + \frac{c}{T^2} \quad (34)$$

where a , b , and c are constants determined from experimental data.

Thompson⁴ has arrived at a significantly improved expression for the heat capacity, viz.,

$$C_p = a + bT + cT^2 + dT^3 + eT^{-2} \quad (35)$$

More generally the heat capacity can be represented by a function which is linear with respect to the parameters, viz.,

$$C_p = \sum_{j=1}^N l_j f_j(T) \quad (36)$$

where the l_j 's are constants* corresponding to the a , b , c 's and the $f_j(T)$'s are pure temperature functions. Equations (34) and (35) are specific cases of Equation (36).

If (36) is substituted into (31) and (32) then

$$H(T) = H(T_b) + \sum_{j=1}^N l_j \int_{T_b}^T f_j(T) dT \quad (37)$$

and

$$S(T) = S(T_b) + \sum_{j=1}^N l_j \int_{T_b}^T \frac{f_j(T)}{T} dT \quad (38)$$

If the integrals in (37) and (38) are defined by:

$$I_j(T) = \int f_j(T) dT \quad (39)$$

$$J_j(T) = \int \frac{f_j(T)}{T} dT \quad (40)$$

*At a given pressure the l_j 's are constant.

then substitution of the limits of integration into (39) and (40) leads to

$$H(T) = H(T_b) - \sum_{j=1}^N l_j I_j(T_b) + \sum_{j=1}^N l_j I_j(T) \quad (41)$$

and

$$S(T) = S(T_b) - \sum_{j=1}^N l_j J_j(T_b) + \sum_{j=1}^N l_j J_j(T) \quad (42)$$

Now if the following definitions are introduced

$$\begin{aligned} l_{N+1} &\equiv H(T_b) - \sum_{j=1}^N l_j I_j(T_b) & (a) \\ I_{N+1} &\equiv 1 & (b) \\ J_{N+1} &\equiv 0 & (c) \end{aligned} \quad (43)$$

$$\begin{aligned} l_{N+2} &\equiv S(T_b) - \sum_{j=1}^N l_j J_j(T_b) & (a) \\ I_{N+2} &\equiv 0 & (b) \\ J_{N+2} &\equiv 1 & (c) \end{aligned} \quad (44)$$

then (41) becomes

$$H(T) = \sum_{j=1}^{N+2} l_j I_j(T) \quad (45)$$

and (42) becomes

$$S(T) = \sum_{j=1}^{N+2} l_j J_j(T) \quad (46)$$

Substitution of (45) and (46) into (33) yields an expression for the free energy.

$$F(T) = \sum_{j=1}^{N+2} l_j K_j(T) \quad (47)$$

where

$$K_j(T) = I_j(T) - T J_j(T) \quad (48)$$

The equations for H, S, and F apply to a single compound in a single phase, i.e., a single species. The l_j 's may be interpreted as elements of a thermodynamic property vector, \vec{I} , which is independent of temperature. The I_j , J_j , K_j may be interpreted as elements enthalpy, entropy and free energy thermal vectors \vec{I} , \vec{J} , \vec{K} , which depend only on temperature and are independent of the compound. The inner product of \vec{I} with \vec{I} , \vec{J} and \vec{K} yield the enthalpy, entropy and free energy, respectively.

Before the above Equations (45), (46), (47) can be of any practical use, the vectors \vec{I} , \vec{J} , \vec{K} and \vec{l} must be evaluated. All of these vectors depend on the linear form chosen to represent the heat capacity data (Equation 36).

In Appendix I, these vectors are calculated using the linear form proposed by Thomson (Equation 35) and thermodynamic property vectors are tabulated for all of the high temperature combustion products for which data are readily available.

2. Multicomponent Systems:

For the i th species in a multicomponent system in which mixing effects are negligible, the enthalpy, entropy and free energy are:

$$H_i = \sum_{j=1}^{N+2} l_{ij} I_j \quad (49)$$

$$S_i = \sum_{j=1}^{N+2} l_{ij} J_j \quad (50)$$

$$F_i = \sum_{j=1}^{N+2} l_{ij} K_j \quad (51)$$

The total enthalpy of the system is:

$$H = \sum_{i=1}^n x_i H_i \quad (52)$$

where x_i is the number of moles of the i th species present in the system and n is the number of species in the system. Similar expressions hold for the total entropy and total free energy of the system. Substitution of (49) into (52) yields:

$$H = \sum_{i=1}^n x_i \sum_{j=1}^{N+2} l_{ij} I_j \quad (53)$$

or in terms of matrices:

$$H = [x_1, x_2, \dots, x_n] \begin{bmatrix} l_{11} & l_{12} & \dots & l_{1,N+2} \\ l_{21} & & & \vdots \\ \vdots & & & \vdots \\ l_{n1} & & & \dots & l_{n,N+2} \end{bmatrix} \begin{bmatrix} I_1 \\ I_2 \\ \vdots \\ I_{N+2} \end{bmatrix} \quad (54)$$

or, more simply:

$$H = X' L I \quad (55)$$

where X' , L and I are the matrices defined by (54) and (55). Similarly, matrix expressions for the total entropy and total free energy of the system may be written:

$$S = X' L J \quad (56)$$

$$F = X' L K \quad (57)$$

The matrix L is seen to be an array of the thermodynamic property vectors of the species present in the system. Henceforth, the matrix L shall be referred to as the thermodynamic property matrix.

Equations (55), (56) and (57) suffer from the fact that mixing effects have been neglected. Mixing can be accounted for by making the following simplifying assumptions:

1. All gaseous species behave ideally.
2. Condensed species have zero enthalpies and entropies of mixing.

For a mixture of ideal gases, the enthalpy of mixing is zero. The entropy of mixing of the i th species, however, is:

$$\Delta S_i = - R \rho_i \quad (58)$$

where

$$\rho_i = \ln x_i + \ln \frac{P}{\bar{x}} \quad (59)$$

Consequently, the corrected entropy and free energy per mole of the i th gaseous species are:

$$\bar{S}_i = S_i - R \rho_i \quad (60)$$

$$\bar{F}_i = F_i + RT \rho_i \quad (61)$$

respectively. These corrected values are also partial molar quantities.

Equations (60) and (61) are applicable to condensed species as well as the gaseous species if it is understood that

$$\rho_i = 0 \quad (62)$$

for all condensed species. Therefore, Equations (49), (60) and (61) may be regarded as being general expressions for the partial molar enthalpy, entropy and free energy of the i th species of a multicomponent system. Substitution of (60) into (50) and (61) into (51), respectively, produces:

$$\bar{S}_i = \sum_{j=1}^N l_{ij} J_j - R \rho_i \quad (63)$$

and

$$\bar{F}_i = \sum_{j=1}^N l_{ij} K_j + RT \rho_i \quad (64)$$

The results of this section can now be applied to the overall specific impulse calculations.

To determine the chamber and exit temperatures it is necessary to be able to evaluate the enthalpy and entropy as functions of temperature and composition (the pressure is given). Equation (55) provides a very simple means of evaluating the enthalpy.

$$H(T, X) = X' L I \quad (55)$$

If Equation (56) is corrected for mixing according to (63), the following matrix equation for evaluating the entropy is obtained:

$$S(T, P, X) = X' [LJ - R\varphi] \quad (65)$$

In Equation (18), which is used to calculate an improved composition convergence, the vectors \mathbf{j}_g and \mathbf{j}_c are required. Both of these vectors can be generated at once by the use of Equation (64) divided by RT. In matrix notation this equation becomes:

$$\begin{matrix} & 1 & N+2 & 1 & 1 \\ n_g \left\{ \begin{bmatrix} \mathbf{j}_g \\ \vdots \\ \mathbf{j}_c \end{bmatrix} \right. & = & \left[\begin{array}{c} L \\ \vdots \\ L \end{array} \right] & \left[\begin{bmatrix} K^* \\ \vdots \\ K^* \end{bmatrix} \right] & + \left[\begin{bmatrix} \varphi_g \\ \vdots \\ \varphi_c \end{bmatrix} \right] \end{matrix} \quad (66)$$

where $K^* = \frac{K}{RT}$

The subscripts g and c refer to the gaseous and condensed species, respectively, and the dimensions of the matrices are designated in the equations by brackets. The vector φ_c is zero.

Equations (55), (65) and (66) are the main results of this section. These equations require that the matrices L, I, J, K, φ and X are given. Elements of the matrix L are independent of temperature, pressure* and composition. For a given problem, therefore, L is invariant. The temperature determines the vectors I, J, K while the pressure and composition determine the vector φ . The vector X, of course, is the composition. Appendix I is concerned with evaluating the vectors I, J, K, and L.

B. Arrangement of the Product Species and the Construction of the Thermodynamic Property Matrix, L.

The matrix L, which is composed of the I vectors, depends on how the I vectors are arranged. Since each I corresponds to one of the product species, the matrix L depends on how the product species are arranged.

In the method for calculating the equilibrium composition described in Section II, a strong distinction was made between

*The elements of L are actually functions of pressure; but at high temperature the variations of the l_{ij} with pressure are probably small.

gaseous species and condensed species. One type of equation was used to describe the gaseous species; another was used to describe the condensed species.

Because of this distinction, care must be exercised in keeping track of in what state each compound finds itself. At a temperature, T , all compounds whose boiling points are less than or equal to T are gaseous, whereas, all compounds whose boiling points are greater than T are condensed. Consequently, as the temperature of a system varies, the number of condensed species may vary.

A general means of treating this problem is to consider all species, i.e., all phases of all compounds, as being present. Each species would be either gaseous or condensed, and the species could be grouped accordingly. Furthermore, these two groups would remain invariant during the course of the solution, regardless of the temperature and pressure. The physical absence of a given species at a given temperature and pressure should be a natural result of the minimization of the free energy, viz., the given species should have an equilibrium composition of zero moles.

This general method, unfortunately, has certain disadvantages. The number of condensed species would always be unnecessarily large so that the difficulties described in Sections II, C 1 and 2, would be accentuated. To overcome these difficulties, it was shown that certain condensed species must be dropped. Consequently, it seems best to consider only those condensed species which are physically present under a given set of conditions, and reject all those which are physically absent. A second disadvantage is that including all species in the problem, whether they be physically present or not, unnecessarily increases the computer storage and time requirements.

The following scheme was employed to distinguish between the various phases. Since all the possible gaseous species are considered, including the gaseous phase of the condensable species, the phase rule only allows one temperature at which both the liquid and solid phase of any one species will exist. This temperature is the melting point, and for the purposes of this discussion the normal melting point will be used. At any given temperature there will be present either the solid or the liquid phase of a condensable species and the gaseous phase.

The method proceeds along the following lines: All the compounds are arranged into two groups, the gaseous and those which are condensed.

It is convenient, therefore, to form two matrices at the beginning of a problem: the L_r matrix and the L_u^* matrix. The L_r matrix is composed of rows corresponding to the r always gaseous compounds; it is invariant during the course of the problem. The L_u^* matrix contains two rows for each condensable compound, one row for each of the liquid and solid phases. At a given temperature one row for each compound is taken from the L_u^* matrix and used to form the L_c matrix which characterizes the thermal properties of the condensable compounds at that temperature. The normal melting point of each compound determines which row of L_u^* is to be used in L_c .

The matrix L which characterizes the thermodynamic properties of the entire system is composed of the two submatrices L_r and L_c .

$$\begin{bmatrix} L \end{bmatrix} = \begin{bmatrix} L_r \\ L_c \end{bmatrix} \quad (67)$$

V. THE COMPUTER PROGRAM FOR CALCULATING THE SPECIFIC IMPULSE

A. Flow Diagram for Calculating the Specific Impulse

Figure 2 is a flow diagram which describes both the overall procedure for calculating the specific impulse and the computer program based on this procedure. The overall procedure may be subdivided into three parts:

- (i) Data handling and preliminary calculations
- (ii) Chamber calculation
- (iii) Equilibrium exhaust calculations

Each row of Figure 2 corresponds to one of these parts. Before the methods for calculating temperatures and compositions can be employed, certain data must be available. These data must be selected, retrieved, and calculated, and as is schematically illustrated by the first row of Figure 2. These computer performed operations are discussed below.

1. Read-in Data

Input data consist of the composition mixture, the chamber and exit pressures, a rough estimate of the chamber temperature, and any necessary instructions needed to modify the number of product species considered. (See Appendix II)

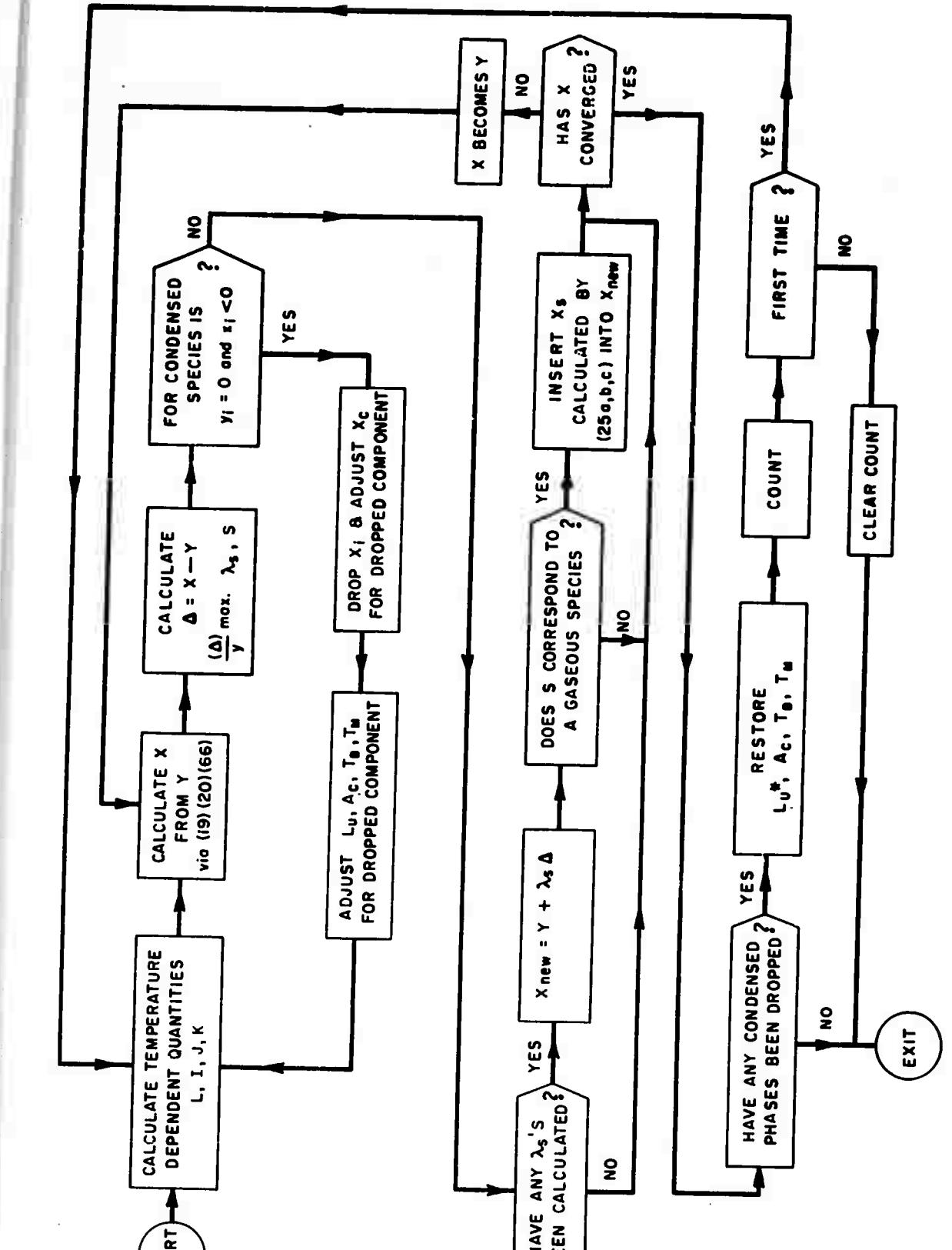


FIG. 2 - Composition Convergence Method

2. What Elements are Present?

A number of predetermined reactants are stored along with their code number, molecular formulas, heats of formation at 298°K., molecular weights, names, and identifying words consisting of the appropriate atomic numbers. This identifying number contains the atomic numbers of all the elements of the compound in ascending numerical order.

3. Construct Reactant Matrices

For each reactant, data are retrieved from the magnetic tape, the Ap and C matrixes are constructed, and a list of each of the following is compiled: molecular weights, heats of formation, and print words for the molecular formulas and names.

4. What Products are Possible?

A number of predetermined products are also stored with their code numbers, formulas, thermodynamic data, molecular weights, melting points, and identifying numbers such as those described for the reactants. Products which contain only those elements present in the fuel mixture are possible species. This is accomplished by comparing the atomic numbers of the elements present, found in part 1 of this discussion, with the atomic numbers in the identifying word. If equality is found, the position of the identifying words in the list is stored as this is the code number of the product.

5. Construct Product Matrices

From the list of code numbers representing the gaseous compounds, the thermodynamic matrix Lr and part of the A matrix are constructed. From the list of code numbers representing the condensed compounds, the thermodynamic matrix Lu* and the remainder of the A matrix are constructed. A melting point vector Tm and a list of the molecular weights of the products are also constructed.

6. Calculate Percent Composition

In this section the input composition, which can be in either moles or grams, is normalized to 100 g. of propellant by the following method.

$$\text{Define } \rho = \frac{\mu}{\sum_{i=1}^p c_i M_i} \quad (68)$$

where $M = 100$ g.

Then the moles of the i th reactant in the system is:

$$r_i = c_{ip} \quad (69)$$

The mole and weight percent of each reactant are computed at this stage of the process also.

If ΔH_{f_i} is the molar heat of formation of the i th reactant and r_i is the number of moles of the i th reactant, then the enthalpy of the reactant system is:

$$\sum_{i=1}^p r_i \Delta H_{f_i}$$

which is also the enthalpy of the products in the chamber. This quantity is calculated by:

$$\sum_{i=1}^p r_i \Delta H_{f_i} = p \sum_{i=1}^p c_i \Delta H_{f_i} \quad (70)$$

To calculate the effects of changes in the heat of formation of the reactants, it is convenient to include two fictitious reactants to the list of propellants. These fictitious reactants have heats of formation of +100 kcal./mole and -100 kcal./mole but no mass. Hence, by including x moles of one of these reactants to a reactant mixture, the heat of formation is increased (or decreased) by $100x$ kcal. and the mass remains unchanged.

7. Store Preliminary Data

The percent composition, formulas and names of the reactants, the formulas of all the products as well as identifying run number are stored on magnetic tape, thereby allowing a large portion of the computer memory to be utilized again.

8. Calculate a Starting Composition

From an element balance the number of gram-atoms of the i th element is given by:

$$b_j = \sum_{i=1}^p a_{ij} r_i \quad (71)$$

where a_{ij} is the number of atoms of element j per molecule of i th reactant. Substitution of equation (69) into (71) gives:

$$b_j = \rho \sum_{i=1}^p a_{ij} r_i \quad (71)$$

where a_{ij} is the number of atoms of element j per molecule of i th reactant. Substitution of equation (69) into (71) gives:

$$b_j = \rho \sum_{i=1}^p a_{ij} c_i \quad (72)$$

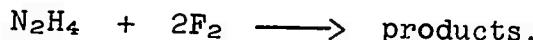
or in matrix notation:

$$B = \rho A_p C \quad (73)$$

Consequently, by using equation (73), all the b_j 's, i.e., the gm.-atoms of all the elements in the system, can be calculated at once.

Example:

For the reaction mixture:



<u>i</u>	<u>j</u>
1 corresponds to N_2H_4	1 corresponds to H
2 corresponds to F_2	2 corresponds to N
	3 corresponds to F

The formula numbers, a_{ij} , the coefficients of the reaction mixture, c_i , and the molecular weights of the reactants, M_i , are given below.

	H			N		F		M_i
	<u>i</u>	a_{11}	a_{12}	a_{13}	c_i			
N_2H_4	1	4	2	0	1			32.048
F_2	2	0	0	2	2			38.00

From equation (68).

$$\rho = \frac{100.0}{32.048 + 2(38.00)}$$

Equation (73) yields:

$$\begin{bmatrix} B \\ \end{bmatrix} = \rho \begin{bmatrix} 40 \\ 20 \\ 02 \end{bmatrix} \begin{bmatrix} 1 \\ 2 \\ \end{bmatrix} = \rho \begin{bmatrix} 4 \\ 2 \\ 4 \end{bmatrix}$$

that is, the system contains 4ρ gram-atoms of H, 2ρ gram-atoms of N, and 4ρ gram-atoms of F. The total weight of the system is 100 g.

The White, Johnson, Dantzig Method requires a starting composition vector Y which is compatible with the element balance. Let Y^o be an arbitrary Y which will be corrected by Y^c so as to make the resulting Y^* compatible with the element balance:

$$\sum_{i=1}^n a_{ij}y_i^* = b_j \quad (74)$$

Substitution of:

$$y_i^* = y^o_i + y_i^c \quad (75)$$

into (74) produces:

$$\sum_{i=1}^n a_{ij}y_i^o + \sum_{j=1}^n a_{ij}c_i = b_j \quad j=1, 2, \dots, m \quad (76)$$

It is desired to determine the y_i^c 's from Equation (76). Since there are but m equations, only m of the y_j 's can be determined from the above equations. Let values of zero, therefore, be assigned to $n-m$ of y_j^c 's so that:

$$\sum_{i=1}^n a_{ij}y_i^o + \sum_{i=1}^m a_{ij}y_i^c = b_j \quad (77)$$

In matrix notation:

$$A' Y^o + A_s' Y^c = B \quad (78)$$

where A_s' is a square $m \times m$ matrix whose columns correspond to m "key" compounds.

Solving (78) for Y^c yields:

$$Y^c = [A_s']^{-1} [B - A' Y^o] \quad (79)$$

where the elements of Y^c correspond to the m key compounds. From (75) and (79) we obtain:

$$Y = Y^o + [A_s']^{-1} [B - A'Y^o] \quad (80)$$

where it is understood that the corrections are added only to the y_i^o 's of the key compounds. Hence, given an arbitrary composition vector Y^o and m key compounds we can calculate a composition vector Y^* which is compatible with the element balance equations.

A convenient choice of Y^o is a vector each element of which is 0.0001 moles. A convenient choice of key compounds are the chemical elements. This choice of "key compounds" eliminates the possibility of negative y_i^* 's.

White, Johnson, and Dantzig have stated that a suitable starting composition, Y^o , must satisfy the mass balance constraints, i.e., Equation (7). They also state that round-off errors in the composition introduced during the course of the calculations can be reduced by using an equation similar to (8). These remarks suggest that compositions which are not compatible with the mass balance constraints have a tendency to make the calculated solutions, i.e., X 's, drift from the true solution.

It has been found, however, that the convergence method, at least for a computer with floating point hardware, is self-stabilizing. In other words, the method will seek out the true solution whether the input composition satisfies the mass balance constraints or not. To verify this point the following numerical experiment was performed on a few problems. First, the equilibrium composition was calculated from a starting composition which agreed with the mass balance constraints. Presumably this equilibrium composition was correct. The same calculation was then repeated except that the starting composition disagreed drastically with the mass balance equations. The equilibrium composition calculated in the second case agreed with the correct equilibrium composition.

Therefore, finding a starting composition which is compatible with the mass balance constraints seems to be an unnecessary operation, although composition convergence is attained much faster if a "correct" starting composition is used.

9. Chamber and Exhaust Solutions

The methods used to obtain both the chamber and exhaust solutions have been extensively discussed in Sections II and III. Figure 2 represents a flow diagram of the method used for computing an equilibrium composition.

10. Storing of Results

All results are stored on magnetic tape as they are obtained. After the problem has been completed, a separate program takes the data from the tape and prints the results. Since the program is automatic, this method of storing the solution saves time by the nature of the speed of writing on magnetic tape versus punching out the answers. A sample output is included in Appendix II.

B. Capabilities of the Computer Program

A program for the Burroughs 220 to calculate the specific impulse has been written according to the method illustrated in Figure 3. The capabilities of this program will now be considered.

A study of Figure 2 reveals that the last operation of a given problem reads in the succeeding problem thereby making the program automatic. Any number of problems may be run without manual intervention. Probable error stops and non-converging solutions are accounted for by a printout, which identifies the difficulty, followed by an instruction to read in the next problem. This scheme enables unattended overnight operation of the program.

Provided that sufficient thermodynamic data are available, the program is general. Computer storage capacity, however, imposes certain restrictions on the size of systems that can be treated. These restrictions are:

- (a) 14 or less reactants in the fuel mixture.
- (b) 12 or less elements in the fuel.
- (c) 12 or less condensed species present in the products or reaction.
- (d) 90 or less products of reaction.

To date all of the problems attempted (over 6000) have remained within these restrictions.

The computer time required to solve one complete problem varies from 3 minutes, for simpler problems, to about 50 minutes for the most difficult problems. Most problems average about 25 minutes of computer time.

Input data for a given problem are kept to a minimum. The selection and preparation of thermodynamic data, as well as all preliminary calculations (such as calculating the gram-atoms of each element in the fuel and enthalpy of the fuel) are performed by the computer. The only input data required are the composition of the reaction mixture, the pressures of the chamber and

nozzle exit, and a rough estimate of the chamber temperature. All other pertinent data are retrieved from magnetic tape where they are permanently stored. The composition of the reaction mixture may be entered either in terms of the fuel compounds (which is usually most desirable), or in terms of the elements and the fuel enthalpy.

An example of input and output from the computer is given in Appendix III.

VI. NOMENCLATURE

A - an $m \times n$ matrix whose elements are a_{ij} for the n products of combustion.

Ac - an $m \times n_c$ matrix whose elements are a_{ij} for the n_c condensed products of combustion.

Ag - an $m \times n_g$ matrix whose elements are a_{ij} for the n_g gaseous products of combustion.

Ap - an $m \times p$ matrix whose elements are a_{ij} for the p propellants.

As - an $m \times m$ matrix whose elements are a_{ij} for the m "key" components used in making a mass balance.

B - an $m \times 1$ column matrix whose elements are b_j .

$C_p(T)$ - the heat capacity at constant pressure as a function of temperature.

C_{pi} - the heat capacity at constant pressure at the temperature T_i , cal./mole/ $^{\circ}$ K.

F_i - the free energy of the i th species, cal./mole.

$F(T)$ - the molar free energy of a compound as a function of temperature, in cal.

$F_r(X)$ - the free energy of a system at a given temperature as a function of the composition X divided by RT.

\mathfrak{F} - an $n \times 1$ column matrix whose elements are \mathfrak{F}_i .

\mathfrak{F}_c - an $n_c \times 1$ column matrix whose elements are the \mathfrak{F}_i for the condensed species.

\mathfrak{F}_i - the ideal partial molal free energy of the i th species divided by RT.

\mathfrak{F}_g - an $n_g \times 1$ column matrix whose elements are the \mathfrak{F}_i for the n_g gaseous species.

G - a function defined by Equation (8).

$H(T)$ - the enthalpy of the system as a function of temperature, in cal.

$H(T, X)$	- the enthalpy of the system as a function of temperature and composition, in cal.
$H(T, X, P)$	- the enthalpy of the system as a function of temperature composition and pressure, in cal.
H_C	- the enthalpy of μ grams of products in the rocket chamber, in cal.
H_E	- the enthalpy of μ grams of products at the rocket exit, in cal.
$H_E(T^\circ)$	- the enthalpy of the elements at the reference temperature, cal./mole.
H_i	- the molar enthalpy of the i th species, in cal./mole.
H_n	- the enthalpy of the system calculated at the temperature, T_n , in cal.
ΔH_{fj}	- the heat of formation at the reactant temperature of the j th reactant, in cal./mole.
I	- the column matrix corresponding to \vec{I} .
I_j	- a function of temperature which is used to describe the enthalpy of a system, units depend on j .
\vec{I}	- the enthalpy thermal vector; a vector whose elements are I_j .
I_{sp}	- the specific impulse, in seconds.
J_j	- a function of temperature which is used to describe the entropy of a system, units depend on j .
J	- the column matrix corresponding to \vec{J} .
\vec{J}	- the entropy thermal vector; a vector whose elements are J_j .
K	- the column matrix corresponding to \vec{K} .
K^*	- K/RT
K_j	- a function of temperature which is used to describe the free energy of a system, units depend on j .

- \vec{K} - the free energy thermal vector; a vector whose elements are K_j .
- L - an $n \times (N+2)$ matrix known as the thermodynamic property matrix; its rows are the \vec{T} 's for all the compounds in the system at a given temperature.
- L_c - an $n_c \times (N+2)$ matrix; its rows are the \vec{T} 's for the n_c condensed species at a given temperature.
- L_u^* - a $3u \times (N+2)$ matrix; its rows are all of the \vec{T} 's for the u condensable compounds.
- L_g - a $r \times (N+2)$ matrix; its rows are the \vec{T} 's for the always gaseous compounds.
- M_i - the molecular weight of the i th species, gm./mole.
- M - an $n \times 1$ column matrix whose elements are M_i .
- N - the number of terms used to characterize the functional dependence of C_p with temperature.
- P - the pressure of the system, in atm.
- P_e - the pressure at the nozzle exit, in atm.
- P_c - the pressure in the rocket chamber, in atm.
- Φ - an $n \times 1$ column matrix whose elements are Φ_i .
- Φ_i - the ideal entropy of mixing of the i th species divided by R.
- Φ_c - an $n_c \times 1$ column matrix whose elements are the entropy of mixing of the n_c condensed species divided by R. This matrix is null.
- Φ_g - an $n_g \times 1$ column matrix whose elements are the Φ_i for n_g gaseous species.

$Q(X)$	- the quadratic approximation to the free energy resulting from a Taylor's Expansion of $F(X)$.
R	- the gas constant per mole, cal./mole/ $^{\circ}$ K.
$S(T, X, P)$	- the entropy of the system as a function of temperature, composition, and pressure, in e.u.
S_i	- the molar entropy of the i th product species, in e.u.
\bar{S}_i	- the partial molar enthalpy of the i th product species, in e.u.
S_c	- the entropy of μ grams of products in the rocket chamber, in e.u.
ΔS_i	- the ideal entropy of mixing of the i th product species, in e.u.
T	- the temperature, $^{\circ}$ K.
T_n	- the n th approximation to a solution temperature.
T_b	- a base temperature, $^{\circ}$ K.
T°	- the reference temperature, $^{\circ}$ K.
X	- an $n \times 1$ vector whose components are x_i .
X_c	- an $n_c \times 1$ column matrix whose components are the x_i for the n_c condensed species.
X_c°	- the equilibrium X at the chamber temperature.
X_e	- the X of the product species at the rocket exit.
X_e°	- the equilibrium X at the rocket exit temperature for equilibrium flow.
X_g	- a $n_g \times 1$ column matrix whose elements are the x_i for the n_g gaseous species.
X_{new}	- $Y + \lambda \Delta$
Y	- an $n \times 1$ column matrix whose components are the y_i .
Y^*	- an $n \times 1$ column matrix whose components, y_i^* , satisfy the mass balance constraints.

y^o - an arbitrary $n \times 1$ column matrix whose elements are y_i^o .

y^c - an $n \times 1$ column matrix whose components are y_i^c .

y_g - an $n_g \times 1$ column matrix whose elements are the y_i for the n_g gaseous species.

y_{gD} - an $n_g \times n_g$ diagonal matrix whose diagonal elements are the y_i for the n_g gaseous species.

a - an empirical constant used to describe heat capacity data.

\vec{a}_i - the formula designation vector; a vector whose elements are $a_{i1}, a_{i2}, \dots a_{im}$.

a_{ij} - a formula designation number which indicates the number of atoms of element j in a molecule of species i .

b - an empirical constant.

b_j - the total number of gm. atomic weights of element j present in the mixture.

c - a constant; in Equation (1) $c = 9.3281 \frac{\text{gm.}^{1/2}}{\text{kcal. sec.}}$

c_i - the number of moles of the i th reactant in the reaction mixture (propellant).

$c(T)$ - the number of condensed compounds in a given system at the temperature T .

d - a constant.

e - a constant.

$f_j(T)$ - a function of temperature used to describe constant pressure heat capacity data.

l_j - empirical constant used to describe thermodynamic properties, see Equations 36, 43 and 44.

\vec{l} - a thermodynamic property vector; a vector whose elements are l_j .

m - the number of chemical elements in a given system.

- n - the total number of product species of a system.
- n_c - the number of condensed product species of the system at a given temperature.
- n_g - the number of gaseous product species of the system at a given temperature.
- p - the number of reactants (propellants).
- r - the number of compounds in a given system which are always gaseous above 1000°K .
- r_j - the number of moles of the j th reactant in the propellant mixture.
- u - the number of condensable compounds in a given system.
- $v(T)$ - the number of vaporized compounds in a given system at the temperature T .
- \bar{x} - the summation of the gaseous x_i .
- $\frac{\bar{x}}{\bar{y}}$ - an $n_g \times 1$ column matrix whose elements are all \bar{x}/\bar{y} .
- x_c - the corrected value of \bar{x} given by (26).
- x_i - the number of moles of the i th product species; x_i is a variable.
- x_s - the number of moles of the s th product species where s identifies the smallest λ , (see Equation 24).
- y_s - the y_i which corresponds to x_s .
- \bar{y} - the summation of the gaseous y_i .
- y_i - the number of moles of the i th product species; y_i is one of the coordinates of Y , a fixed point about which a Taylor's Expansion is made.
- y_i^* - the number of moles of the i th species; an element of Y^* .
- y_i° - an arbitrary number of moles of the i th species.
- y_i^c - $y_i^* - y_i^\circ$.

- α - an $m \times 1$ column matrix whose elements are α_j .
- α_j - the atomic weight of the j th element.
- λ - a scale factor which reduces the step length given by Δ . See Equation (23).
- λ_i - the largest λ which prevents x_i from becoming negative.
- λ_s - the smallest of all the λ_i .
- μ - the mass of the propellant system, in gms.
- π - an $m \times 1$ vector whose elements are the π_j 's.
- π_j - a Lagrange multiplier associated with the mass balance equation for the j th element.
- $\bar{\pi}$ - a vector whose elements are the π_j .
- ρ - the number of reaction weights in a system of mass μ .
- δ_k - a constant multiplier.
- ϕ_H - a factor used in estimating improved temperatures when enthalpy is used in the convergence criterion.
- ϕ_s - a factor used in estimating improved temperatures when entropy is used in the convergence criterion.
- Δ - an $n \times 1$ column matrix or vector which indicates the directions toward an improved solution X-Y.
- Δ_i - an element of Δ , $x_i - y_i$.

Subscripts

- c - chamber conditions; condensed species.
- e - exit conditions.
- g - gaseous species.
- i - a dummy index usually used to designate a species.
- j - a dummy index usually used to designate a chemical element.

k - a dummy index.

Superscripts

/ - denotes the transpose of a matrix.
-1 - denotes the inverse of a matrix.

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VIII. APPENDICES

APPENDIX I

THE THERMODYNAMIC PROPERTY VECTORS OF THE COMBUSTION PRODUCTS

The general formulation of the thermodynamic property vectors given in Section IV is now applied using the heat capacity expression suggested by Thomson⁴ and the thermodynamic property data compiled by The Dow Thermal Laboratory.⁵ The thermodynamic property vectors resulting from the above source are tabulated at the end of this Appendix.

The constant pressure heat capacity expression proposed by Thomson is of the form:

$$C_p = l_1 + l_2 + l_3 T^2 + l_4 T^3 + l_5 T^{-2} \quad (81)$$

where T is the temperature in °K., divided by 1000 and the l_i 's are constants to be determined from experimental measurements.

Following the method prescribed by Thomson, the constants l_1 through l_5 were calculated from values of the heat capacity measured at five characteristic temperatures. If T_1 to T_5 and C_{p1} to C_{p5} are the characteristic temperatures and their corresponding heat capacities, respectively, then (81) leads to the following matrix equation:

$$\begin{bmatrix} C_{p1} \\ C_{p2} \\ C_{p3} \\ C_{p4} \\ C_{p5} \end{bmatrix} = \begin{bmatrix} 1 & T_1 & T_1^2 & T_1^3 & T_1^{-2} \\ 1 & T_2 & T_2^2 & T_2^3 & T_2^{-2} \\ 1 & T_3 & T_3^2 & T_3^3 & T_3^{-2} \\ 1 & T_4 & T_4^2 & T_4^3 & T_4^{-2} \\ 1 & T_5 & T_5^2 & T_5^3 & T_5^{-2} \end{bmatrix} \begin{bmatrix} l_1 \\ l_2 \\ l_3 \\ l_4 \\ l_5 \end{bmatrix} \quad (82)$$

Solving for unknowns l_i 's gives:

$$\begin{bmatrix} l_1 \\ l_2 \\ l_3 \\ l_4 \\ l_5 \end{bmatrix} = \begin{bmatrix} 1 & T_1 & T_1^2 & T_1^3 & T_1^{-2} \\ 1 & T_2 & T_2^2 & T_2^3 & T_2^{-2} \\ 1 & T_3 & T_3^2 & T_3^3 & T_3^{-2} \\ 1 & T_4 & T_4^2 & T_4^3 & T_4^{-2} \\ 1 & T_5 & T_5^2 & T_5^3 & T_5^{-2} \end{bmatrix}^{-1} \begin{bmatrix} C_{p1} \\ C_{p2} \\ C_{p3} \\ C_{p4} \\ C_{p5} \end{bmatrix} \quad (83)$$

where \mathbf{T} is the square matrix of Equation (82). For species not undergoing phase changes, the five characteristic temperatures are:

1000, 1600, 3000, 4500, and 5700°K.

However, if a phase change did occur, then five temperatures with spacings proportional to those above were chosen so as to cover the complete temperature range of each phase. (Table III contains the temperature range used in calculating the l_j 's for each compound.) Equation (83), therefore, is used to calculate l_1 through l_5 .

The quantities l_6 and l_7 are calculated according to (43a) and (44a):

$$l_6 = H(T_b) - \sum_{j=1}^5 l_j I_j(T_b) \quad (43a)$$

$$l_7 = S(T_b) - \sum_{j=1}^5 l_j J_j(T_b) \quad (44a)$$

Before these expressions can be applied, the functions H , S , I , and J must be evaluated at $T = T_b$.

Absolute entropies are generally obtainable, but absolute enthalpies are not.* Consequently, $S(T_b)$, in (44a), is the absolute entropy at the base temperature, T_b , while $H(T_b)$, in (43a), must be a relative enthalpy. A convenient reference state for evaluating enthalpies is the elements at standard conditions. If this reference state is chosen then:

$$H(T_b) = [H(T_b) - H(T^\circ)] + [H(T^\circ) - H_E(T^\circ)] \quad (74)$$

Both of the bracketed terms on the right side of (74) are available from the Thermodynamic Tables⁶. The first term is the change in enthalpy in going from the reference temperature, T° , to the base temperature, T_b , while the second term is the heat of formation from the elements at T° . The entropy at the base temperature, $S(T_b)$, is also available from the Thermodynamic Tables.⁶

The functions I and J are defined by Equations (39) and (40).

$$I_j(T) = \int f_j(T) dT \quad (39)$$

$$J_j(T) = \int \frac{f_j(T)}{T} dT \quad (40)$$

The above integrations are straightforward and are given in Table II.

* This stems from difficulties in measuring the zero point energy.

[†] This reference state is especially useful in treating multi-component systems since it is independent of the composition.

TABLE II
Elements of the Thermal Vectors

J	$f_j(T)$	$I_j(T)$	$J_j(T)$	$K_j(T)$
1	1	T	$\ln T$	$T(1-\ln T)$
2	T	$1/2 T^2$	T	$-1/2 T^2$
3	T^2	$1/3 T^3$	$1/2 T^2$	$-1/6 T^3$
4	T^3	$1/4 T^4$	$1/3 T^3$	$-1/12 T^4$
5	T^{-2}	$-T^{-1}$	$-1/2 T^{-2}$	$-3/2 T^{-1}$
6	-	1	0	1
7	-	0	1	-T

Hence, from $H(T_b)$ calculated via (84), $S(T_b)$ obtained from the Thermodynamic Tables⁶, and $I_j(T_b)$ and $J_j(T_b)$ calculated from Table II, l_6 and l_7 can be evaluated using (43a) and (44a).

Study of Equation (31) or (32) reveals that T_b must be chosen within the temperature range for which l_1 through l_5 are valid. Choosing a T_b outside this range is satisfactory only if l_1 through l_5 represent the behavior of C_p versus T to the temperature T_b . This condition, however, does not generally prevail. Because of slight variations between the observed heat capacity data and those predicted from l_1 through l_5 , slight variations in l_6 and l_7 occur if T_b is allowed to vary. Therefore, rather than choose l_6 and l_7 corresponding to a given T_b , it seems best to calculate the average values of l_6 and l_7 based on several T_b 's. Values of l_6 and l_7 entered in Table III are the arithmetic means of l_6 and l_7 calculated at T_b 's equal to the five characteristic temperatures described above.

By itself the thermodynamic property vector l has little significance; it must be associated with the enthalpy thermal vector, I, the entropy thermal vector, J, or the free energy thermal vector, K, before it takes on real significance. The elements of these thermal vectors are listed in Table II. Notice that f_1 through f_5 are defined by (81), I_j and J_j for $j=6$ and 7 are defined by (43) and (44) and the K_j 's are defined by (48).

Using the procedure outlined above, the elements (l_1 through l_7) of the thermodynamic property vectors of 98 combustion products have been calculated. The results of these calculations are entered in Table III below.

Values of C_p , H, and S generated from the thermodynamic property vectors in Table III agree with the tabulated values⁶ to better than 1 per cent.

TABLE III
 The Thermodynamic Property Vectors of the Combustion Products

Compound	State	1 ₁ , cal. mole ⁻¹ deg.	1 ₂ , cal. mole ⁻¹ deg. ⁻²	1 ₃ , cal. mole ⁻¹ deg. ⁻³	1 ₄ , cal. mole ⁻¹ deg. ⁻⁴	1 ₅ , cal. mole ⁻¹ deg.	1 ₆ , cal. mole ⁻¹ deg.	1 ₇ , cal. mole ⁻¹ deg.
H ₂	Gas	5.744149	1.635989	-0.248476	.016153	.072174	-1.448891	38.230614
L ₁	Gas	2.457282	1.640946	-0.429329	.055169	2.002388	40.618854	38.573728
Liquid		-2.418100	14.759800	-8.639400	1.747200	1.440980	4.451267	6.252650
B _e	Gas	5.699850	-.5233923	.075088	.010273	.281289	75.642194	78.908278
Liquid		7.502100	-.001300	.000180	-.000033	-.000300	-9511992	10.374975
Solid		-11.240600	28.868500	-16.846900	3.763280	1.985610	7.375959	-11.981354
B	Gas	4.835241	.138751	-.049714	.005982	.039740	132.840500	42.564906
Liquid		7.500060	-.000050	.000001	-.000001	-.000110	.150016	8.229363
Solid		6.307720	.276890	.150920	-.007161	-.829511	-.083689	5.832890
C	Gas	4.955040	-.115265	.088130	-.008817	.050912	169.491930	43.376216
Solid		5.952581	.090093	.047520	-.004650	-.945554	-.137887	5.36328
N ₂	Gas	7.929263	.590846	-.108108	.007366	-.609376	-.671440	53.670058
O ₂	Gas	7.801681	.736242	-.044113	-.001623	-.151897	-.285733	57.08590
F ₂	Gas	8.917622	.170069	.002042	-.000356	-.239384	-.363338	58.142316
Na	Gas	5.457544	-.261398	-.022043	.023565	-.263275	23.800082	42.863912
Liquid		14.614400	-18.224200	14.797300	-.3.852600	-.405500	-.285798	34.428566
Mg	Gas	6.563759	-.1.000133	.1.162329	.008449	-.994329	31.998526	41.963526
Liquid		5.259000	2.600000	-.011000	.001000	-.001000	.456393	15.704905
Al	Gas	2.228060	1.673550	-.392564	.032841	3.088500	80.624890	45.009532
Liquid		6.999970	-.000020	-.000010	.000002	.0000021	.320119	17.525313
S ₁	Gas	3.585831	1.187848	-.244481	.016644	.464457	104.928180	45.462232
Liquid		7.000032	-.000014	.000003	-.000000	-.000000	7.959939	17.816459
Solid		4.009400	2.841300	-.871300	.124770	-.240270	-.846493	9.073350
P	Gas	4.317574	.141874	-.07145	.002034	-.034158	19.913882	30.959438

TABLE III (cont'd.)

Compound	State	$l_1, \text{cal. mole}^{-1} \text{deg.}^{-1}$	$l_2, \text{cal. mole}^{-1} \text{deg.}^{-2}$	$l_3, \text{cal. mole}^{-1} \text{deg.}^{-3}$	$l_4, \text{cal. mole}^{-1} \text{deg.}^{-4}$	$l_5, \text{cal. mole}^{-1} \text{deg.}^{-5}$	$l_6, \text{cal. mole}^{-1} \text{deg.}^{-6}$	$l_7, \text{cal. mole}^{-1} \text{deg.}^{-7}$
S	Gas	4.429339	.059446	-.007343	.000563	-.072050	13.859881	32.248750
Cl ₂	Gas	8.381033	.091746	.008968	-.000572	-.120860	-3.046699	63.560914
AlCl ₃	Gas	9.005825	.053504	.012649	-.001072	-.100901	-.12.566050	61.355124
AlCl ₃	Gas	20.160797	-.238597	.062530	-.005176	-.429413	-.145.569230	96.359028
AlF	Gas	8.897665	.099776	.001728	-.000569	-.175698	-.63.703580	61.305636
AlF ₃	Gas	19.780051	.062389	-.015326	.001297	-.578400	-.291.450500	61.277874
AlF ₃	Solid	20.944700	2.971400	.013900	-.002300	-.001800	-.362.401500	35.626656
AlH	Gas	8.631479	.336546	-.034554	.002323	-.565797	57.759176	53.-01928
Al ₂ O	Gas	13.578075	.183637	-.036000	.002276	-.867991	-.43.533577	73.707984
AlO	Gas	8.950356	.055608	.010295	-.001042	-.285214	12.366667	61.797460
Al ₂ O ₃	Liquid	³⁴ 9.999000	.000600	-.000100	.000010	.001400	-.794.469800	51.719042
Al ₂ O ₃	Solid	30.368400	-1.342800	2.257200	-.265520	-.1.098570	-.113.211740	42.870188
B ₂	Gas	8.931215	.099802	.002568	-.000269	-.323296	196.850980	97.767184
BCl	Gas	8.9245361	.086346	.001781	-.000203	-.223274	41.-671-E	60.771380
BCl ₃	Gas	19.766962	.063183	-.014245	.001120	-.707035	-.105.651510	90.048176
BF	Gas	8.686775	.225412	-.031870	.002250	-.422567	-.46.833594	56.800514
BF ₃	Gas	19.335961	.316310	-.066960	.004814	-.1.460134	-276.604480	78.350340
BH	Gas	7.974582	.678720	-.111491	.007834	-.709845	112.351420	48.823348
BN	Gas	8.619241	.269865	-.048039	.004705	-.475376	120.526820	52.995974
BN	Solid	11.079684	.871314	-.200260	.026036	-.1.231697	-67.113745	11.657726
B ₂ O ₂	Gas	19.879583	.534709	-.109022	.007902	-.1.583249	-114.749510	78.260484
BO	Gas	8.419721	.349223	-.055905	.004854	-.587694	6.670053	56.958908

APPENDIX II

INPUT

Input data for a given problem consist of:

- (i) A test word which indicates whether the input is in moles or grams, and whether a modification in the number of product species is to be considered.
- (ii) The propellant composition designated by two numbers. The first number is the number of moles or grams of the given reactant in the reaction mixture and the second number identifies the reactant.
- (iii) The chamber and exit pressures.
- (iv) A rough estimate of the chamber temperature.
- (v) An identifying run number.
- (vi) Any appropriate changes in the melting points of the condensable species.
- (vii) Any modification of the product species.

Figure 3 is a sample input sheet for a lithium aluminum hydride-nitronium perchlorate-polyethylene system. The pressures and temperature are given in floating decimal number.

There is also included the output data sheet obtained from the input (Figure 4).

Fig. 3 - Sample Input for Specific Impulse Calculation

Test word

Fuels

P_c
P_e
T_c
Run No.

Melting Point Change

6	30	0495	-

8

6	04	4956
.	.	.
.	.	.
.	.	.
.	.	7
.	.	.
.	.	.
.	.	.
.	.	.
.	.	7a
.	.	.
.	.	.
.	.	.
.	.	.
.	.	7b
.	.	.
.	.	.
.	.	.
.	.	.
.	.	7c
.	.	.
.	.	.
.	.	.
.	.	.
.	.	7d
.	.	.
.	.	.
.	.	.
.	.	.
.	.	7e

Run Number 5736

No. Products 58 No. Gases 51 No. Condensed Phases 4

Percent			
Mole	Weight	Formula	Name
29.40	18.00	LiAlH ₄ -S	Lithium Aluminum Hydride
26.42	62.00	ClNO ₆ -S	Nitronium Perchlorate
44.19	20.00	C ₂ H ₄ -S	Polyethylene

 ΔF_{298}°

Species	Chamber Moles	Exhaust Moles	Exhaust Grams
Al	.001737		
AlCl	.010421		
AlClO	.000019		
AlCl ₂	.003354		.000001
AlCl ₃	.000008		
AlH	.000438		
AlHO	.000021		
AlHO ₂	.001975		
AlN	.000001		
AlO	.000635		
Al ₂ O	.002284		
Al ₂ O ₂	.000022		
HCN	.000156	.000003	.000086
CHNO	.000007		.000005
CHO	.001283	.000009	.000264
CH ₂ O	.000021		.000012
CH ₄	.000002		.000007
CN	.000006		
CO	1.394454	1.370447	38.387588
CO ₂	.029877	.055330	2.435122
Cl	.003279	.000003	.000101
HCl	.075704	.008211	.299418
HOCl	.000001		
LiCl	.328966	.402002	17.043689
Cl ₂	.000001		
Li ₂ Cl ₂	.000544	.007995	.677887
Li ₃ Cl ₃		.000002	.000208
H	.123172	.000919	.000926
LiH	.009217	.000107	.000850
LiOH	.082462	.054228	1.298659

Fig. 4 - Output Data Sheet

Run Number 5736 (Continued)

Species	Chamber Moles	Exhaust Moles	Exhaust Grams
NH	.000037		
OH	.008881	.000009	.000156
H ₂	1.897070	2.032152	4.096817
H ₂ O	.325619	.310483	5.593658
Li	.048864	.001925	.013361
LiN	.003041	.000016	.000333
LiO	.000422		.000004
Li ₂ O	.000108	.000002	.000064
N	.000008		
NO	.000361		.000002
N ₂	.211302	.213100	5.970205
O	.000333		
O ₂	.000023		
Al ₂ O _{3-s,l}	.225530	.237142	24.178961
Temperature, °K.	3278.838	1781.701	
Pressure, atmos.	68.046	1.000	
Enthalpy, kcal.	-17.288	-113.398	
Entropy, e.u.	267.536	267.542	
Moles of gas	4.566	4.457	
Avg. mol. wt., g.	16.864	17.011	
Gamma	1.271	1.297	
Velocity, cm./sec.		283601.740	
Impulse, sec.		289.182	

Fig. 4 (Contd.)

Appendix III

Constants for the Generation of Thermodynamic Properties

		<u>1₇</u>	<u>1₁</u>	<u>1₂</u>	<u>1₃</u>	<u>1₄</u>	<u>1₅</u>	<u>1₆</u>
1	Al-s,1							
Liquid	.313024	6.999998		-.000002				17.505829
Solid	-1.405771	4.509173	3.726023	-.395728	.056896	.030096		11.293808
2	Al							
Gas	76.676926	4.776660	.251993	-.105005	.012815	.034967		45.190472
3	AlC							
Gas	207.166560	8.936989	.003666	-.000649	.000029	-.038166		64.836556
4	AlCl							
Gas	-14.515948	8.927057	.128628	-.002432	.000183	-.069447		54.650864
5	AlClF							
Gas	-127.842500	13.822715	.058575	-.013266	.000969	-.221203		83.207030
6	AlClF ₂							
Gas	-242.387820	19.654005	.143912	-.032649	.002457	-.470776		92.167426
7	AlClO							
Gas	-60.434504	14.743334	.106130	-.024068	.001606	-.319903		75.654400
8	AlCl ₂							
Gas	-82.622110	13.873462	.025127	-.005930	.000467	-.148151		85.510600
9	AlCl ₂ F							
Gas	-188.891440	19.741701	.086295	-.019562	.001471	-.369535		95.940084
10	AlCl ₃ -s,1							
Liquid	-171.260020	32.000014	-.000010	.000010	-.000001	-.000002		79.316950
Solid	-175.139200	21.494140	3.303880	-.057440	.002047	.000239		51.664118
11	AlCl ₃							
Gas	-147.229740	19.795746	.052108	-.012092	.0000926	-.275726		97.712420

Constants for the Generation of Thermodynamic Properties (Contd.)

		<u>17</u>	<u>16</u>	<u>15</u>	<u>14</u>	<u>13</u>	<u>12</u>	<u>11</u>	<u>10</u>
12	AlF								
Gas	-64.437528	8.844102	.156476	-.015131	.001147	-.154175	61.262344		
13	AlFO								
Gas	-126.894180	14.657329	.162297	-.0366673	.002746	-.470914	71.226150		
14	AlF ₂								
Gas	-162.176490	13.747689	.106437	-.023870	.001773	-.332791	77.708208		
15	AlF _{3-s}								
Solid	-364.485000	23.030046	.472470	1.060943	-.148793	-.435725	41.273244		
16	AlF ₃								
Gas	-293.140800	19.512428	.239812	-.054846	.004147	-.595287	85.914286		
17	AlH								
Gas	58.548288	8.016235	.759065	-.134423	.010026	-.238854	53.253478		
18	AlHO								
Gas	-10.091417	13.521079	.903354	-.203669	.015229	-.822436	63.538370		
19	AlHO ₂								
Gas	-115.792090	15.958609	2.337450	-.500433	.036253	-.609940	76.326640		
20	LiAlO _{2-s,l}								
Solid	-293.046520	22.057610	2.945100	-.032810	.008017	-.598256	35.181416		
21	AlN-s								
Solid	-79.647272	8.885381	4.186307	-.731181	.001142	-.243969	13.168159		
22	AlN								
Gas	101.326920	8.816987	.195019	-.019385	.001471	-.167959	64.091422		
23	AlNaO ₂								
Solid	-288.517760	36.590060	-23.166150	16.147530	-3.213257	-1.809068	58.656186		
24	AlO								
Gas	14.154399	8.752837	.207667	-.028478	.002142	-.195455	61.724172		

Constants for the Generation of Thermodynamic Properties (Contd.)

				<u>1₇</u>	<u>1₁</u>	<u>1₂</u>	<u>1₃</u>	<u>1₄</u>	<u>1₅</u>	<u>1₆</u>
25	AlS ₁									
Gas	65.998922	8.903370	.120445	-.006091	.000466	-.105032	65.272192			
26	Al ₂ Cl ₆									
Gas	-323.176700	43.594463	.082839	-.018824	.001415	-.557589	167.293000			
27	Al ₂ MgO ₄									
Solid	-550.545980	36.811190	6.383990	.007240	-.000937	-.979208	56.402300			
28	Al ₂ O									
Gas	-44.902828	13.488140	.280113	-.063833	.004813	-.463210	75.546296			
29	Al ₂ O ₂									
Gas	-113.545420	20.093349	.506919	-.114507	.008572	-.709317	82.241378			
30	Al ₂ O ₃ -s,1									
Liquid	-353.572260	-2.954006	33.937299	-9.912413	.942705	1.186401	27.576094			
Solid	-412.873800	28.590178	3.510857	-1.250880	.140219	-1.176349	39.578596			
31	Al ₂ O ₅ S1									
Solid	-669.998620	40.055870	5.926070	-.043380	.009098	-1.010293	63.987954			
32	Al ₄ C ₃									
Solid	-65.339212	43.665350	3.372740	-.071990	.008985	-1.063709	70.848058			
33	B-s,1									
Liquid	-333478	7.265811	.300591	-.088045	.007555	-.574260	8.138727			
Solid	-2.203576	4.282623	2.819016	-.798698	.078112	-.251056	4.450282			
34	B									
Gas	131.172050	4.910933	.076806	-.033186	.004591	.006847	42.603302			
35	BCl									
Gas	40.062010	8.820411	.167809	-.016775	.001259	-.165320	60.735858			
36	BClF									
Gas	-83.213296	13.087646	.539613	-.122070	.009154	-.475521	76.643810			

Constants for the Generation of Thermodynamic Properties (Contd.)

		<u>1₇</u>	<u>1₁</u>	<u>1₂</u>	<u>1₃</u>	<u>1₄</u>	<u>1₅</u>	<u>1₆</u>
37	BClF ₂							
Gas	-219.840100	18.740476	.739276	-.166538	.012439	-.814008	84.473538	
38	BOCl							
Gas	-90.087446	13.599501	.838962	-.187430	.013935	-.376467	71.417936	
39	BCl ₂							
Gas	-24.610648	13.720012	.125898	-.028470	.002127	-.279028	80.550048	
40	BCl ₂ F							
Gas	-161.836720	19.130728	.487693	-.110449	.0038287	-.674250	88.337232	
41	BCl ₃							
Gas	-104.704350	19.489910	.252036	-.057133	.004287	-.556545	89.964366	
42	BF							
Gas	-48.737594	8.357616	.455160	-.086278	.006462	-.245859	56.710808	
43	BOF							
Gas	-148.585490	13.407415	.965814	-.216333	.016119	-.516564	67.573500	
44	BF ₂							
Gas	-139.321510	13.117458	.519330	-.117390	.008799	-.492219	72.376776	
45	BF ₃							
Gas	-278.449440	18.336059	1.004078	-.226506	.016943	-.934649	77.990752	
46	BH							
Gas	112.239560	6.995424	1.367169	-.270654	.019985	-.126461	48.570182	
47	BOH							
Gas	-52.515988	11.617090	2.095887	-.466533	.034635	-.590683	59.193072	
48	HOBO							
Gas	-141.994860	13.915040	3.582615	-.770552	.055989	-.763678	69.387450	

Constants for the Generation of Thermodynamic Properties (Contd.)

		<u>1₇</u>	<u>1₁</u>	<u>1₂</u>	<u>1₃</u>	<u>1₄</u>	<u>1₅</u>	<u>1₆</u>
49	BH ₂							
Gas	61.436400	10.084665	2.429497	- .539523	.039996	- .474133	56.511172	
50	BH ₂ O ₂							
Gas	-53.721498	18.347725	4.530856	- .977580	.071147	- .973413	79.036864	
51	BH ₃							
Gas	12.700039	10.020179	6.105641	-1.336416	.098161	- .675542	52.164544	
52	H ₃ BO ₃							
Gas	-251.814180	26.146019	7.053549	-1.525544	.111213	-1.631083	87.711905	
53	NaBH ₄ -s,1							
Solid	-67.409946	47.485580	-31.931620	19.944650	-4.067810	-2.915957	76.437216	
54	BN-s							
Solid	-66.851758	11.261024	.598636	- .100663	.006426	-1.023995	12.186024	
55	BN							
Gas	148.521330	8.217253	.546445	- .106420	.007949	- .245461	59.350364	
56	NaBO ₂ -s,1							
Liquid	-240.046300	28.409067	1.153760	- .473244	.065541	-1.140955	46.623770	
Solid	-237.080920	11.600070	13.999840	.0000050	- .000059	- .000006	27.433676	
57	BO							
Gas	.796945	7.660478	.866139	- .183943	.013690	- .206819	56.693806	
58	BS							
Gas	67.207352	8.590891	.287221	- .052261	.003909	- .230482	60.842274	
59	B ₂							
Gas	196.030040	8.699155	.262340	- .035955	.002679	- .211418	57.636122	

Constants for the Generation of Thermodynamic Properties (Contd.)

		<u>17</u>	<u>11</u>	<u>12</u>	<u>13</u>	<u>14</u>	<u>15</u>	<u>16</u>
60	B_2O_4							
Gas	-130.449870	30.141483	.436143	-.098996	.007457	-.918935	117.122610	
61	B_2He							
Gas	-10.268054	27.946582	9.983782	-2.212206	.163718	-2.914923	72.329126	
62	B_2O_2							
Gas	-119.563840	18.029968	1.823048	-.407451	.030310	-.799606	74.653442	
63	$B_2O_3-s,1$							
Liquid	-318.104840	33.376392	-1.272985	.373093	-.031186	-2.782318	48.006302	
Solid	-280.626320	-65.924870	199.075130	-127.073663	26.734663	3.953444	-100.183890	
64	B_2O_3							
Gas	-221.311840	21.347133	2.892342	-.647421	.048203	-1.513369	82.007612	
65	$B_3Cl_3O_3$							
Gas	-423.214480	47.357105	1.525525	-.344919	.025838	-2.209970	129.124690	
66	$B_3F_3O_3$							
Gas	-589.178280	46.963580	1.786232	-.404218	.030296	-2.553608	121.858300	
67	$B_3H_3O_6$							
Gas	-568.137380	54.494210	7.814724	-.1.674013	.121297	-3.103061	130.900150	
68	$B_3H_6N_3$							
Gas	-150.514570	45.215270	13.729205	-2.989808	.218921	-3.845194	100.866120	
69	$B_4C-s,1$							
Liquid	-1.900567	29.510904	.421625	-.121948	.010631	-1.232141	41.224142	
Solid	-25.487032	25.540513	6.263060	-2.722480	.376390	-1.709618	26.876722	
70	$Na_2B_4O_7-s,1$							
Liquid	-827.583020	87.553550	4.229260	-.300350	.134505	-5.830977	121.215510	
Solid	-797.653320	27.099780	57.999800	-.000200	-.000030	.000005	60.807426	

Constants for the Generation of Thermodynamic Properties (contd.)

		<u>1₇</u>	<u>1₁</u>	<u>1₂</u>	<u>1₃</u>	<u>1₄</u>	<u>1₅</u>	<u>1₆</u>
71	BeH_9	-20.670278	55.509220	15.255991	-3.390231	.251344	-5.938271	99.917626
Gas								
72	$\text{B}_{10}\text{H}_{14}$	-60.494198	103.348080	22.743120	-5.053538	.374644	-10.065773	153.632870
Gas								
73	Be-s,1	1.098488	4.7666792	2.244073	-.568624	.045512	-.388090	8.742361
Liquid								
Solid		-1.725879	4.607906	1.724538	.340273	-.061700	-.072130	6.833384
74	Be	76.394542	5.018807	.013976	-.068346	.022217	-.010871	38.568546
Gas								
75	BeC_2	128.889160	12.332072	1.644152	-.366160	.027173	-.758501	61.367740
Gas								
76	BeCl	33.818630	8.829016	.168060	-.016974	.001273	-.166241	61.694032
Gas								
77	BeClF	-130.262980	14.360690	.356315	-.080378	.006009	-.617626	70.078278
Gas								
78	BeCl_2	-86.033954	14.581060	.213180	-.048439	.003645	-.405249	73.367652
Gas								
79	BeF	1.525062	8.511206	.362150	-.064690	.004874	-.237679	58.203498
Gas								
80	BeF_2	-189.168040	13.905903	.652467	-.147193	.011014	-.695429	65.498250
Gas								
81	BeH	74.533868	7.460431	1.0888219	-.209795	.015539	-.187259	50.111682
Gas								

Constants for the Generation of Thermodynamic Properties (Contd.)

		<u>1₇</u>	<u>1₁</u>	<u>1₂</u>	<u>1₃</u>	<u>1₄</u>	<u>1₅</u>	<u>1₆</u>
82	BeHO							
Gas	-44.952074	9.334943	2.682100	-.567772	.040837	-.244789	62.190978	
83	BeH ₂							
Gas	23.836242	11.289797	2.327007	-.520486	.038733	-.880755	50.237890	
84	BeH ₂ O ₂							
Gas	-165.684580	16.141763	6.386887	-.1.368356	.099171	-1.261378	64.896484	
85	BeO-s,1							
Liquid	-127.925810	-.791018	12.844814	-.3.135429	.245308	.530452	8.255100	
Solid	-148.287520	10.726526	2.133544	-.550426	.054482	-.588126	12.655268	
86	BeO							
Gas	27.199116	8.261953	.512788	-.100278	.007515	-.246050	55.903880	
87	Be ₂ C							
Liquid	-12.348956	19.500016	-.000024	-.000002				
Solid	-24.094008	5.389302	17.203406	-.5.987984	.687804	-.147513	28.569150 6.210096	
88	Be ₂ Cl ₄							
Gas	-199.512790	29.976862	1.196290	-.270883	.020314	-1.744455	93.079212	
89	Be ₂ O ₂							
Gas	-110.915340	18.683342	.795030	-.184122	.014118	-.925398	77.771712	
90	Be ₃ N ₂ -s,1							
Liquid	-116.447000	34.999996	.000005					
Solid	-142.102940	22.067825	13.611458	-.3.078478	-.003661	-.000001	54.980300 29.847476	
91	Be ₃ O ₈							
Gas	-274.948220	29.404571	1.570326	-.355216	.0266616	-2.000817	89.410432	

Constants for the Generation of Thermodynamic Properties (Contd.)

		<u>1₇</u>	<u>1₁</u>	<u>1₂</u>	<u>1₃</u>	<u>1₄</u>	<u>1₅</u>	<u>1₆</u>
92	Be ₄ O ₄							
Gas	-397.881920	40.530396	2.093584	-.473440	.035467	-2.694566	107.304050	
93	Be ₅ O ₅							
Gas	-519.812840	51.653150	2.620631	-.593058	.044462	-3.387942	124.530420	
94	Be ₆ O ₆							
Gas	-662.844080	62.773790	3.149658	-.712988	.053463	-4.081012	141.350760	
95	C-S							
Solid	-3.236550	5.364067	.454333	-.093518	.008848	-.518240	5.193956	
96	C							
Gas	169.321130	5.128910	-.256669	.124645	-.011837	-.014314	43.969762	
97	CCL							
Gas	128.892930	8.831985	.104301	-.016420	.001234	-.147797	63.690944	
98	CClFO							
Gas	-110.083420	18.211480	1.076220	-.241617	.018022	-.825362	83.794622	
99	CClF ₅							
Gas	-176.074850	24.635770	.789295	-.178995	.013444	-1.164086	91.881968	
100	CClN							
Gas	27.105596	12.993748	1.226510	-.270344	.020060	-.369982	69.961118	
102	CCl ₂ F							
Gas	-75.162512	25.299489	.351537	-.079429	.005942	-.811056	100.328400	

Constants for the Generation of Thermodynamic Properties (Contd.)

		<u>1₇</u>	<u>1₁</u>	<u>1₂</u>	<u>1₃</u>	<u>1₄</u>	<u>1₅</u>	<u>1₆</u>
103	CCl ₄							
Gas	-35.665472	25.539650	.194668	-.044259	.003330	-.649833	101.4777910	
104	CF							
Gas	71.129452	8.472163	.390032	-.069975	.005152	-.235639	59.906204	
105	CFN							
Gas	-8.274402	12.748741	1.371245	-.304816	.022606	-.451247	66.727922	
106	CF ₂							
Gas	-51.754364	12.979625	.703464	-.138361	.010374	-.592516	70.016770	
107	CF ₂ O							
Gas	-159.467480	17.807903	1.336454	-.299813	.022353	-.985744	78.125662	
108	CF ₃							
Gas	-138.473010	18.500594	.898134	-.202963	.015210	-.926457	79.881582	
109	CF ₄							
Gas	-229.517360	24.221224	1.059553	-.239855	.017990	-1.344073	84.758022	
110	CH							
Gas	139.998010	6.324556	1.724714	-.347737	.025417	-.019289	50.825316	
111	CHClF ₂							
Gas	-122.410320	21.214349	2.878290	-.631814	.046481	-1.262587	85.010592	
112	CHCl ₂ F							
Gas	-71.004078	21.642003	2.600818	-.569803	.041885	-1.091300	90.020426	
113	CHCl ₃							
Gas	-34.603932	21.996968	2.366056	-.516379	.037859	-.928909	91.921538	
114	CHFO							
Gas	-97.595732	14.852859	3.137170	-.690039	.050837	-.975824	71.324160	

Constants for the Generation of Thermodynamic Properties (Contd.)

		<u>1₇</u>	<u>1₁</u>	<u>1₂</u>	<u>1₃</u>	<u>1₄</u>	<u>1₅</u>	<u>1₆</u>
115	CHF ₃							
Gas	-173.383280	20.828625	3.129198	-.688270	.050696	-1.418625	79.391084	
116	HCN							
Gas	26.979230	9.986136	3.250734	-.651461	.047056	-1.353130	57.630370	
117	CHNO							
Gas	-34.228678	14.074463	3.496895	-.753186	.054768	-.631866	69.814306	
118	CHO							
Gas	-7.112880	9.605640	2.664107	-.5822820	.042800	-.403585	62.660910	
119	CH ₂							
Gas	62.118256	8.103459	4.147580	-.899150	.065644	-.423667	49.848576	
120	CH ₂ ClF							
Gas	-67.546064	18.009842	4.832264	-1.055696	.077455	-1.274683	77.370188	
121	CH ₂ Cl ₂							
Gas	-31.652748	18.513698	4.503238	-.981407	.071891	-1.131238	80.140592	
122	CH ₂ F ₂							
Gas	-115.409340	17.547138	5.145811	-1.127498	.082862	-1.438133	71.740404	
123	CH ₂ O							
Gas	-34.505852	12.186877	4.805755	-1.057404	.077920	-968787	61.108172	
124	CH ₃							
Gas	26.003928	11.262893	5.356246	-1.174951	.086414	-765771	54.645838	
125	CH ₃ Cl							
Gas	-29.120522	15.007863	6.654601	-1.449382	.106124	-1.204770	66.286470	
126	CH ₃ Cl ₃ S ₁							
Gas	-135.288130	22.600720	21.427670	-9.356010	1.541070	-.389553	103.161430	

Constants for the Generation of Thermodynamic Properties (Contd.)

		<u>1₇</u>	<u>1₁</u>	<u>1₂</u>	<u>1₃</u>	<u>1₄</u>	<u>1₅</u>	<u>1₆</u>
127	CH ₃ F							
Gas	-67.769140	14.474479	7.021297	-1.534494	.112604	-1.350646	62.361040	
128	CH ₃ FeS ₁							
Gas	-303.126620	19.301320	27.139140	-13.214180	2.491270	-5.004655	88.204722	
129	CH ₄							
Gas	-25.160290	11.661670	8.707460	-1.895976	.138799	-1.120690	50.904648	
130	MgCO ₃ -s							
Solid	-274.237580	20.595900	8.073000	6.261000	-2.478000	-5.06930	35.143878	
131	CN							
Gas	88.510436	7.388968	.633676	.165751	.028860	-1.17159	56.488444	
132	NaCN-s,1							
Liquid	-24.594028	20.999990	.000009	.000003	.000002	.000002	57.671954	
Solid	-25.763984	13.000050	10.000100	-.000030	.000050	-.000002	42.693906	
133	NaCN							
Gas	26.555690	12.999997	.00001				83.144004	
134	NaCO ₃ -s							
Liquid	-284.473240	47.388440	.979640	-.375560	.048656	-1.512106	82.488554	
Solid	-337.696440	140.162560	-180.285920	120.392550	-24.306690	-10.633385	199.996480	
135	CO							
Gas	-29.109842	7.263554	1.103525	-.235811	.017634	-.159392	54.979636	
136	CO ₂							
Gas	-38.669236	13.154942	1.277352	-.249812	.018566	-.511373	68.338456	
137	CO ₂							
Gas	-99.623754	12.226062	1.789351	-.380132	.029171	-.590839	62.475718	

Constants for the Generation of Thermodynamic Properties (Contd.)

		<u>1₇</u>	<u>1₁</u>	<u>1₂</u>	<u>1₃</u>	<u>1₄</u>	<u>1₅</u>	<u>1₆</u>
138	CP	89.705870	8.542839	.314457	-.058855	.004402	-.236227	60.769028
Gas	CS	68.206246	8.497865	.339804	-.065295	.004871	-.240513	59.329988
140	CS ₂	22.298244	14.072677	.576108	-.121729	.009092	-.462859	71.388380
Gas	CS ₁ -S	-17.705031	9.996904	1.786304	.019390	-.004791	-.368576	13.438009
141	CTH-s,1	-30.742006	12.699697	.000001	.019606	-.003139	.0000001	24.182002
Liquid	Solid	-48.579372	11.854710	.761283	.019606	-.003139	-.362467	17.906981
142	C ₂	195.956190	6.792445	1.805289	-.355200	.023236	.314701	57.044328
Gas	C ₂ F ₂	-59.057580	18.844614	1.2698102	-.290015	.021591	-.662207	79.407850
144	C ₂ F ₄	-165.024010	29.023056	1.803639	-.405821	.030311	-1.459301	99.846168
Gas	C ₂ H ₂	48.649000	12.704947	5.180604	-1.038340	.075106	-.482764	59.438028
146	C ₂ H ₄	2.124806	17.412427	8.809391	-1.914535	.139984	-1.547497	63.5222214
Gas	C ₂ H ₄ O	-26.119568	22.585753	9.333424	-2.034061	.149000	-2.184897	72.119502

Constants for the Generation of Thermodynamic Properties (Contd.)

		<u>1₇</u>	<u>1₁</u>	<u>1₂</u>	<u>1₃</u>	<u>1₄</u>	<u>1₅</u>	<u>1₆</u>
149	$\text{Li}_2\text{C}_2-\text{s}$							
Solid	-24.005082	24.469500	2.204310	.136620	-.025576	-.720667	38.911014	
150	MgC_2-s							
Solid	14.648259	17.017755	1.544050	-.000750	-0000355	-.359886	31.108470	
151	CaN_2							
Gas	66.657956	17.113022	2.381911	-.528647	.039168	-.644429	74.606248	
152	C_3							
Gas	184.069830	12.648416	1.442686	-.321489	.023872	-.565843	62.829372	
153	$\text{Mg}_2\text{C}_3-\text{s}$							
Solid	8.384323	28.440140	2.447860	.067780	-.013221	-.604847	54.289946	
154	C_3O_2							
Gas	-18.172851	22.241892	2.925825	-.651268	.048335	-1.088006	81.967940	
155	C_4							
Gas	234.143060	17.609287	2.082690	-.464036	.034450	-.810482	74.832162	
156	$\text{C}_4\text{H}_{12}\text{S}_1-\text{s}$							
Gas	-77.822886	15.438710	80.784800	-33.627600	5.108230	-.438265	80.040874	
157	C_4N_2							
Gas	115.734160	27.050822	3.649160	-.810554	.060071	-1.125970	95.466932	
158	C_5							
Gas	232.218640	22.570146	2.722714	-.606584	.045028	-1.055122	80.965504	
159	Cl							
Gas	27.253020	5.613747	-.400034	.087661	-.006445	.000290	46.317924	
160	ClF							
Gas	-16.858370	9.227216	-.305960	.158624	-.015773	-.194730	62.326988	
161	Li_2ClF							
Gas	-187.751950	19.611524	.174089	-.039865	.003010	-.524196	84.962408	

Constants for the Generation of Thermodynamic Properties (Contd.)

		<u>1₇</u>	<u>1₁</u>	<u>1₂</u>	<u>1₃</u>	<u>1₄</u>	<u>1₅</u>	<u>1₆</u>
162	MgClF							
Gas	-144.231910	14.833033	.048156	-.011131	.000851	-.276860	76.087262	
163	FeClO ₃							
Gas	-16.303092	24.454744	.906356	-.205192	.015390	-.1.214639	89.864412	
164	ClF ₃							
Gas	-46.241098	19.704880	.111571	-.025393	.001908	-.458640	89.414902	
165	SiClF ₃							
Gas	-325.062320	25.384624	.297081	-.067448	.005066	-.771485	100.383770	
166	HCl							
Gas	-23.844752	6.169057	1.765351	-.361643	.026302	.009848	51.680660	
167	HOC1							
Gas	-25.889486	10.092730	2.218470	-.466771	.033430	-.249864	66.866336	
168	SiClH ₃							
Gas	-58.344798	19.992095	3.724137	-.828455	.061457	-.1.349683	76.421038	
169	NH ₄ Cl							
Solid	-111.439760	69.180130	-59.364580	32.632400	-6.178204	-6.220941	96.310762	
170	NH ₄ ClO ₄							
Solid	-91.810294	70.699200	.005000	.003000	-.001000	-.000040	126.053420	
171	LiCl-s,1							
Liquid	-97.666966	14.400003	-.000009	-.000001	-.000001	-.000001	33.526212	
Solid	-100.931150	10.616830	4.695360	.037440	-.023284	-.048198	23.512954	
172	LiCl							
Gas	-46.830008	8.896482	.163814	-.007491	.000576	-.114148	60.951110	

Constants for the Generation of Thermodynamic Properties (contd.)

		<u>17</u>	<u>11</u>	<u>12</u>	<u>13</u>	<u>14</u>	<u>15</u>	<u>16</u>
173	LiOCl							
Gas	-8.807584	13.517402	.258785	-.058547	.004284	-.429426	75.369930	
174	LiClO ₄ -s,1							
Liquid	-98.730764	32.819880	19.999900					
Solid	-100.771170	29.022300	27.483000	-.018000	-.000020	-.000019	68.886424	56.617998
175	MgCl							
Gas	-1.879457	8.927568	.125591	-.002714	.000215	-.064429	66.139730	
176	NOCl							
Gas	7.658387	12.698095	1.149883	-.176049	.013119	-.360167	75.803460	
177	NaCl-s,1							
Liquid	-97.989990	16.000006	.000002	-.000004			39.582498	
Solid	-101.682250	10.979990	3.899990	-.000010	-.000009	-.000001	29.437456	
178	NaCl							
Gas	-46.863648	8.937650	.181807	-.000970	.000086	-.042580	65.407850	
179	ClO							
Gas	21.013860	8.815760	.194330	-.019091	.000131	-.169833	63.890566	
180	ClO ₂							
Gas	19.467665	13.422319	.495070	-.072557	.005437	-.477099	75.159688	
181	SiCl							
Gas	45.287602	8.931160	.099835	-.001465	.000101	-.044681	67.241234	
182	TiCl							
Gas	14.119456	8.933987	.196907	-.000992	.000054	-.063300	69.221068	
183	Cl ₂							
Gas	-3.230782	9.366107	-.439384	.213974	-.021676	-.143300	64.013784	

Constants for the Generation of Thermodynamic Properties (Contd.)

			<u>1₇</u>	<u>1₁</u>	<u>1₂</u>	<u>1₃</u>	<u>1₄</u>	<u>1₅</u>	<u>1₆</u>
184	SiH ₂ Cl ₂								
Gas	-85.086738	21.900065	2.509708		-.558830		.041460	-.1.092863	88.845210
185	Li ₂ Cl ₂								
Gas	-147.930820	19.772043	.065829		-.014743		.001092	-.376854	89.530432
186	MgCl ₂ -s,1								
Liquid	-151.568010	22.100008	-.000016		.000008			.000001	54.758430
Solid	-159.748630	19.244470	.689390		.5000160		-.109636	-.227634	43.279108
187	MgCl ₂								
Gas	-105.745610	14.864795	.026150		-.005921		.000444	-.186362	78.467794
188	Cl ₂ O								
Gas	12.889794	13.667817	.160710		-.036491		.002741	-.352598	78.336520
189	SiCl ₂								
Gas	-42.383474	13.872430	.023724		-.004982		.000344	-.179023	82.853848
190	TlCl ₂ -s,1								
Liquid	-124.948920	21.000003	-.000020					.52.103068	
Solid	-128.120350	16.599980	3.000010		-.000020		-.000005	-.000001	42.687330
191	TlCl ₂								
Gas	-77.698016	13.999996	.000003						76.012244
192	ZrCl ₂ -s,1								
Liquid	-147.543990	23.000007	.000014		-.000007			.000003	57.281598
Solid	-150.317900	17.299960	4.200000		-.000020		-.000019	-.000001	46.760344
193	ZrCl ₂								
Gas	-96.333818	15.907852	.001115		-.000026		-.000014	-.056351	84.843278
194	SiCl ₃ F								
Gas	-210.131140	25.636362	.130848		-.029572		.002207	-.455918	108.868700

Constants for the Generation of Thermodynamic Properties (Contd.)

		<u>1₇</u>	<u>1₁</u>	<u>1₂</u>	<u>1₃</u>	<u>1₄</u>	<u>1₅</u>	<u>1₆</u>
195	Si HCl ₃							
Gas	-121.573570	23.698517	1.359496	-.302122	.022392	-.766885	99.269572	
196	Li ₃ Cl ₃							
Gas	-240.264560	31.526010	.179545	-.040961	.003092	-.785982	114.150210	
197	POCl ₃							
Gas	-144.165550	25.293918	.354533	-.080113	.005996	-.625478	104.612360	
198	PCl ₃							
Gas	-69.275700	19.825066	.030886	-.006890	.000512	-.262213	97.126332	
199	PCl ₅							
Gas	-100.135510	25.701542	.088422	-.020260	.001537	-.449471	109.196850	
200	TiCl ₃ -S							
Solid	-180.089850	24.274450	1.874650	1.226700	-.236886	297210	60.616036	
201	TiCl ₃							
Gas	-138.004080	19.071326	.199797	-.005033	.000434	-.165006	96.979876	
202	ZrCl ₃ -S,1							
Liquid	-209.882980	31.500006	-.000002	-.000001			79.172676	
Solid	-214.957760	21.399980	12.999930	-.000130	-.000020	-.000001	56.521636	
203	ZrCl ₃							
Gas	-160.216070	19.860821	.007328	-.001627	.000124	-.149026	105.716900	
204	SiCl ₄							
Gas	-154.775230	25.720683	.075622	-.017281	.001307	-.428836	108.067540	
205	TiCl ₄							
Gas	-191.06630	25.784611	.031029	-.006583	.000462	-.296885	113.788330	

Constants for the Generation of Thermodynamic Properties (Contd.)

		<u>17</u>	<u>11</u>	<u>12</u>	<u>13</u>	<u>14</u>	<u>15</u>	<u>16</u>	<u>17</u>
206	ZrCl ₄ -s,1								
Liquid	-241.517040	40.000020	-.0000010	.0000010	.0000010	-.000003	97.224636		
Solid	-241.593960	31.913700	.009020	-.004052	.000562	-.290319	81.484200		
207	ZrCl ₄								
Gas	-216.073080	25.802179	.021222	-.004771	.000357	-.232411	117.655970		
208	PCl ₅								
Gas	-95.914434	31.686962	.072341	-.016485	.001245	-.557542	118.282210		
209	F								
Gas	17.539261	5.070510	-.0666876	.015150	-.001136	.060321	44.365718		
210	HF								
Gas	-65.661692	5.385666	2.006661	-.285756	.026779	.169273	48.254026		
211	HOF								
Gas	-30.029304	9.880022	2.356958	-.498094	.035785	-.283613	63.919390		
212	SiH ₃ F								
Gas	-115.678170	19.827898	3.831330	-.852566	.063251	-1.471835	72.756042		
213	LiF-s,1								
Liquid	-145.285970	15.310006	-.000006	-.000002					
Solid	-144.507140	1.793866	19.137859	-8.605517	1.252471	.615758	8.215178		
214	LiF								
Gas	-82.502574	8.794453	.234800	-.022511	.001696	-.179610	57.483638		
215	LiOF								
Gas	-15.564964	13.420635	.321702	-.072686	.005439	-.488749	72.546926		
216	MgP								
Gas	-24.082146	8.881695	.132800	-.009070	.000681	-.132728	62.871228		

Constants for the Generation of Thermodynamic Properties (Contd.)

		1 ₇	1 ₁	1 ₂	1 ₃	1 ₄	1 ₅	1 ₆
217	NF	55.364266	8.750545	.127583	-.029119	.002200	-.196583	58.458050
218	FNO	-20.878960	12.617978	.835367	-.187304	.013961	-.440396	72.144164
219	NaF-s,1							
Liquid	-136.143960	16.400009	-.000013	-.000001				
Solid	-139.736280	10.531951	3.581420	.208253	-.034607	-.040103	33.246772	23.700488
220	NaF							
Gas	-69.971412	8.912101	.116940	-.005034	.000393	-.094841	61.943768	
221	OF							
Gas	29.164712	8.749673	.128706	-.029563	.002253	-.196479	60.299150	
222	PF							
Gas	-20.220200	8.779595	.178038	-.024213	.001820	-.187947	63.347863	
223	PSF							
Gas	-46.290746	13.665276	.162989	-.037241	.002812	-.377454	80.896422	
224	S1F							
Gas	7.204554	8.828964	.152530	-.016764	.001256	-.144049	63.865276	
225	F ₂							
Gas	-3.215851	8.791140	.307074	-.022521	.001695	-.183065	58.069530	
226	S1H ₂ F ₂							
Gas	-205.091220	21.203976	2.966383	-.661769	.049177	-1.482719	79.834293	
227	Li ₂ F ₂							
Gas	-221.400500	19.520489	.232408	-.052659	.003945	-.642756	81.509030	

Constants for the Generation of Thermodynamic Properties (contd.)

		<u>1₇</u>	<u>1₁</u>	<u>1₂</u>	<u>1₃</u>	<u>1₄</u>	<u>1₅</u>	<u>1₆</u>
228	MgF ₂ -s,1							
Liquid	-260.151000	22.570001	.000008	-.000001		.000001	42.687156	
Solid	-268.551180	16.997741	2.445019	.023267	-.001731	-.228963	32.199366	
229	MgF ₂							
Gas	-182.557060	14.767466	.091712	-.021131	.001610	-.354662	71.858886	
230	R ₂₀							
Gas	2.206879	13.634567	.181763	-.041176	.003088	-.412886	73.475292	
231	SiO ₂ F ₂							
Gas	-121.039570	19.158875	.470548	-.106893	.008042	-.723669	85.942742	
232	SiO ₂ F ₂							
Gas	-160.972990	24.367317	.961483	-.217340	.016282	-1.156690	91.757116	
233	PF ₂							
Gas	-114.272180	13.680987	.153426	-.035236	.002677	-.370057	76.810306	
234	SiF ₂							
Gas	-123.493740	13.463370	.293605	-.066350	.004668	-.463302	74.612542	
235	TlF ₂ -s,1							
Liquid	-217.344960	21.000001	.000003	-.000004		-.000001	45.293066	
Solid	-222.398000	13.700010	7.000000	.000003	-.000003	-.000002	32.484894	
236	TlF ₂							
Gas	-137.392540	13.582158	.217959	-.049644	.0035739	-.418517	79.459434	
237	ZrF ₂ -s,1							
Liquid	-229.324940	29.999994	-.000002	-.000001			59.809414	
Solid	-236.281920	19.399950	11.200000	.000010	-.000010	-.000002	41.138682	

Constants for the Generation of Thermodynamic Properties (Contd.)

		<u>17</u>	<u>11</u>	<u>12</u>	<u>13</u>	<u>14</u>	<u>15</u>	<u>16</u>
238	ZnF ₂							
Gas	-151.709700	13.805820	.069629	-.015864	.001195	-.274455	76.564646	
239	SiHF ₃							
Gas	-293.624140	23.024656	1.798295	-.400895	.029775	-1.166076	87.847566	
240	Li ₃ F ₃							
Gas	-370.856320	30.934584	.5666333	-.128061	.009579	-1.253769	101.958210	
241	NF ₃							
Gas	-38.116320	19.281557	.389141	-.088142	.006613	-.829480	81.254630	
242	PF ₃							
Gas	-228.649720	19.467715	.268232	-.061011	.004591	-.664787	85.199578	
243	TlF ₃ -s,1							
Liquid	-332.425940	28.000013	-.000019	-.000002			59.894000	
Solid	-340.827040	17.200030	11.200010	.000010	-.000004		39.473978	
244	TlF ₃							
Gas	-263.131520	19.586070	.189882	-.043217	.003254	-.613904	88.723248	
245	ZrF ₃ -s,1							
Liquid	-347.424880	31.999986	-.000002	-.000004			69.872858	
Solid	-357.096860	22.400006	9.399970	-.000006			51.253888	
246	ZnF ₃							
Gas	-278.295380	19.755502	.076867	-.017315	.001292	-.398942	92.054550	
247	SiF ₄							
Gas	-383.472280	25.041120	.523246	-.118631	.008902	-.967048	92.657644	
248	TlF ₄ -s							
Solid	-398.869340	15.399900	40.003800	-.003700	.000800	.000070	38.728878	

Constants for the Generation of Thermodynamic Properties (Contd.)

		<u>1₇</u>	<u>1₁</u>	<u>1₂</u>	<u>1₃</u>	<u>1₄</u>	<u>1₅</u>	<u>1₆</u>
249	TlF ₄							
Gas	-379.3988060	25.486691	.229323	-.051973	.003897	-.676461	101.604580	
250	ZnF ₄ -s,1							
Liquid	-447.898100	18.098098	23.820150	-10.815635	1.583001	.369465	53.548232	
Solid	-470.102400	33.278999	.121270	-.095903	-.002194	-1.083846	59.782562	
251	ZnF ₄							
Gas	-408.547500	25.644064	.127194	-.029240	.002225	-.521908	105.168300	
252	SR ₆							
Gas	-304.713320	36.929326	.546311	-.123944	.009294	-1.605729	105.867520	
253	H							
Gas	50.621310	4.967999	.000002					33.404515
254	LiH							
Gas	28.814984	8.375470	.579567	-.082492	.006138	-.247350	49.619288	
255	LiOH-s,1							
Liquid	-120.235960	20.740000	-.000010	-.000002	.000001	-.000001	36.633790	
Solid	-116.818910	1.264480	31.574950	-16.308700	2.80367	.469782	5.229932	
256	LiOH							
Gas	-61.685642	9.744508	2.399972	-.502415	.035875	-.315344	62.165864	
257	MgH							
Gas	37.440840	8.300312	.526014	-.095072	.007133	-.247611	54.867620	
258	MgOH							
Gas	-16.072417	10.062525	2.244506	-.473492	.033376	-.247413	68.047888	

Constants for the Generation of Thermodynamic Properties (Contd.)

		<u>1₇</u>	<u>1₁</u>	<u>1₂</u>	<u>1₃</u>	<u>1₄</u>	<u>1₅</u>	<u>1₆</u>
259	NH							
Gas	77.566954	5.871481	1.935644	-.387239	.027959	.062003	50.161504	
260	NaH							
Gas	26.579168	8.613321	.445306	-.048135	.003587	-.228348	54.179236	
261	NaOH-s,1							
Liquid	-105.062170	19.083680	.840108	-.266859	.028207	.324866	41.996290	
Solid	-121.630220	43.420390	-36.858360	21.190120	-4.145827	-2.950127	65.767932	
262	NaOH							
Gas	-59.081066	10.088060	2.212412	-.464186	.033176	-.172592	67.620396	
263	OH							
Gas	8.059381	5.539488	2.029926	-.402411	.028569	.147895	50.760544	
264	PH							
Gas	52.385620	6.986268	1.355447	-.271294	.020027	-.124918	54.421950	
265	HS							
Gas	32.826868	6.534243	1.598349	-.324816	.023830	-.054298	54.536912	
266	SiH							
Gas	111.162000	7.455745	1.110821	-.211426	.015711	-.187816	55.279614	
267	H ₂							
Gas	-1.059953	5.290330	2.024190	-.352047	.024860	.193870	37.936122	
268	LiO ₂ H ₂							
Gas	-181.136920	22.944479	5.142059	-1.082201	.077536	-1.479650	78.737222	
269	MgH ₂ -s							
Solid	-25.955370	18.420552	-10.860800	7.613660	-1.766407	-.929447	28.149334	

Constants for the Generation of Thermodynamic Properties (contd.)

			<u>17</u>	<u>18</u>	<u>19</u>	<u>12</u>	<u>13</u>	<u>14</u>	<u>15</u>	<u>16</u>	<u>17</u>
270	MgO ₂ H ₂ -S	Solid	-227.729360	18.469400	9.650000	5.625000	-1.764700	-1.85570	32.937540		
271	NH ₂	Gas	37.989890	6.726628	4.233935	-0.898776	.064741	-.047498	51.859186		
272	H ₂ O	Gas	-59.597646	6.083043	1.625610	-0.933442	.066088	.061312	51.465054		
273	H ₂ O ₂	Gas	-37.707634	12.720020	2.893730	-0.090740	-.104430	-.392794	68.163596		
274	H ₂ SO ₄ -1	Liquid	-201.987400	24.230540	37.989140	-24.396200	5.114660	.233648	57.407636		
275	PH ₂	Gas	35.032030	9.835376	2.576715	-0.570582	.042213	-.450341	59.875316		
276	SiH ₂	Gas	-8.507971	8.625942	3.434304	-0.716336	.052611	-.320397	57.138274		
277	NH ₃	Gas	-14.645140	7.831464	7.080605	-1.501533	.108113	-.323726	51.928286		
278	H ₃ PO ₄ -S,1	Liquid	-313.661120	48.000070	.000050	.000030	-.000020	-.000006	96.387798		
		Solid	-343.298120	114.656700	-231.981200	267.058400	-104.969500	-4.765040	198.603180		
279	PH ₃	Gas	-.813127	13.276554	4.181543	-.927203	.068639	-.1.007777	60.333502		
280	N ₂ H ₄	Gas	16.611584	14.543000	7.096630	3.062790	-1.892760	-.430086	69.863322		

Constants for the Generation of Thermodynamic Properties (Contd.)

		<u>1₇</u>	<u>1₁</u>	<u>1₂</u>	<u>1₃</u>	<u>1₄</u>	<u>1₅</u>	<u>1₆</u>
281	SiH ₄							
Gas	-2.632605	18.153918	4.897658	-1.089702	.080843	-1.550359	61.926646	
282	Li-s,1							
Liquid	-1.314616	7.080335	-.382112	.140542	-.016171	.069401	17.120514	
Solid	-2.508972	7.615058	-.569250	.327251	-.064031	-.045563	15.763572	
283	Li							
Gas	36.834498	5.103289	-.104315	-.026272	.024037	-.019892	39.259726	
284	LiN							
Gas	35.809592	8.175167	.577669	-.113739	.008488	-.239407	59.326202	
285	LiO							
Gas	10.723379	8.400532	.427013	-.080422	.006031	-.244172	58.890424	
286	Li ₂							
Gas	47.590724	8.934596	.329650	-.001462	.000114	-.039268	57.548064	
287	Li ₂ O-s,1							
Liquid	-139.174930	23.000002	-.000006	-.000004			37.694352	
Solid	-148.440750	14.899548	6.160570	-.056622	.013316	-.335083	23.286554	
288	Li ₂ O							
Gas	-39.796262	13.396744	.336936	-.075968	.005672	-.533482	69.464822	
289	Li ₃ N-s							
Solid	-55.316516	17.993510	22.945670	-15.237300	3.254832	-.458482	21.952540	
290	Mg-s,1							
Liquid	.419915	5.277602	2.619245	-.007666	.000917	-.010106	15.684376	
Solid	-.477917	2.770681	6.585290	-1.723270	.345766	.202559	10.270231	

Constants for the Generation of Thermodynamic Properties (Contd.)

		<u>17</u>	<u>11</u>	<u>12</u>	<u>13</u>	<u>14</u>	<u>15</u>	<u>16</u>
291	Mg	33.877512	4.892170	.179632	-.136045	.030886	.004041	41.397328
292	MgO-s							
Solid	-148.140390	11.347224	1.716498	-.592647	.073251	-.303114	18.068232	
293	MgO							
Gas	1.062427	8.853366	.157550	-.013162	.000976	-.149994	60.839506	
294	MgSiO ₃ -s,1							
Liquid	-371.495360	33.808258	3.115617	-.963576	.100105	-2.888419	47.614966	
Solid	-373.301040	26.150450	2.400660	1.177697	-.191592	-.797808	42.723856	
295	MgSO ₄ -s,1							
Liquid	-326.346760	20.707960	25.186680	-9.960350	1.341266	-4.313216	35.813154	
Solid	-311.168600	15.891410	25.264440	-1.042340	.230260	.027015	34.396660	
296	MgS-s							
Solid	-85.873318	9.250017	2.500014	-.000009	-.000001	-.000001	21.436704	
297	MgS							
Gas	30.278596	8.925893	.010396	-.002190	.000154	-.079891	67.7E2430	
298	Mg ₂ SiO ₄ -s,1							
Liquid	-523.605200	48.133940	3.986890	-1.237206	.12694	-3.927548	67.543390	
Solid	-527.086320	36.356300	5.676470	.381230	-.037642	-.903778	59.993932	
299	Mg ₂ Si-s,1							
Liquid	-7.500006	22.500008	-.000005	.000001			56.789540	
Solid	-24.610466	17.418627	3.572550	.209790	-.115220	-.193236	38.392312	
300	Mg ₃ N ₂ -s							
Solid	-120.3733970	27.630730	4.580040	-2.838140	.531852	-.704426	50.367150	

Constants for the Generation of Thermodynamic Properties (Contd.)

		<u>1_r</u>	<u>1₁</u>	<u>1₂</u>	<u>1₃</u>	<u>1₄</u>	<u>1₅</u>	<u>1₆</u>
301	Mg ₃ P ₂ O ₈ -s,1							
Liquid	-933.258320	92.371880	4.472330	-1.404660	.147706	-6.006343	126.407850	
Solid	-911.157640	45.330990	38.461980	2.060570	-.304130	-.584794	85.125750	
302	N							
Gas	111.392770	5.104901	-.136980	.022207	.004887	-.018643	42.745226	
303	NO							
Gas	18.744525	7.674605	.862283	-.182096	.013546	-.193729	58.524526	
304	NO ₂							
Gas	2.359917	12.486581	.927845	-.208851	.015597	-.623810	69.166918	
305	PN							
Gas	18.308411	8.436739	.377472	-.074813	.005604	-.242868	59.380122	
306	NS							
Gas	59.851228	8.567751	.306864	-.056203	.004228	-.189166	62.444114	
307	SiN							
Gas	117.712610	8.623190	.269171	-.047745	.003589	-.225573	61.049006	
308	TiN-s,1							
Liquid	-69.266994	13.499997	.000002	-.000001			25.826828	
Solid	-85.086192	11.904955	.937349	.005190			19.659744	
309	ZrN-s,1							
Liquid	-73.462376	11.127090	2.321936	-.584313	.046595	-.223952	26.593178	
Solid	-91.263454	11.109331	1.677631	.000619	-.000049	-.172326	21.251010	
310	N ₂							
Gas	-2.486823	6.973146	1.274237	-.274263	.020277	-.118559	53.318418	

Constants for the Generation of Thermodynamic Properties (Contd.)

		<u>17</u>	<u>14</u>	<u>12</u>	<u>10</u>	<u>12</u>	<u>10</u>	<u>14</u>	<u>12</u>	<u>10</u>	<u>15</u>	<u>16</u>
311	N ₂ O											
Gas	13.859506	12.615769	1.462495		-.325805		.024187		-.580897		64.571162	
312	N ₂ O ₃											
Gas	9.886999	23.191949	1.713949		-.384981		.028722		-1.058318		96.363930	
313	N ₂ O ₄											
Gas	-11.238626	28.519676	2.129959		-.479038		.035767		-1.567590		98.829954	
314	N ₂ O ₅											
Gas	-13.515669	34.026953	2.429875		-.547112		.040884		-2.012556		106.216730	
315	S ₁₃ N ₄ -s											
Solid	-179.842690	4.311000	49.454320		-16.292290		1.772628		.860841		18.286594	
316	P ₃ N ₅ -s											
Solid	-78.645180	12.270630	61.678170		-28.015910		4.101365		.912413		46.613850	
317	Na-s,1											
Liquid	-2.815188	11.280620	-10.314610		7.643958		-.1.562591		-.134248		29.556202	
Solid	-2.464839	7.999940	.000100		-.001100		.000210		.000002		21.739644	
318	Na											
Gas	24.980838	3.778455	1.631630		-.728519		.107934		.135597		41.472904	
319	NaO											
Gas	10.158282	8.892911	.160650		-.007379		.000555		-.118115		64.151816	
320	Na ₂											
Gas	30.155478	8.946818	.380721		.001285		-.000116		-.009121		65.657172	

Constants for the Generation of Thermodynamic Properties (Contd.)

		<u>17</u>	<u>11</u>	<u>12</u>	<u>13</u>	<u>14</u>	<u>15</u>	<u>16</u>
321	Na ₂ O-s,1							
Liquid	-100.379550	23.999995	-.000011	.000002				
Solid	-104.320940	15.699980	5.400000	-.000010	-.000014			
322	Na ₂ SiO ₃ -s,1							
Liquid	-369.413760	43.115911	.852509	-.257077	.026179	-2.022543	75.737758	
Solid	-373.132140	31.862120	7.855460	1.511900	-.444850	-.690584	59.608388	
323	Na ₂ Si ₂ O ₂ -s,1							
Liquid	-596.710080	62.450930	4.449350	-1.365656	.141253	-.4.869901	100.672420	
Solid	-590.015580	44.520390	16.608960	.073310	.045920	-1.077288	82.447956	
324	Na ₂ S-s,1							
Liquid	-95.772686	21.913349	.169723	-.079770	.009960	-.4.10187	48.339782	
Solid	-94.529958	18.099970	3.000030	-.000020	-.000009		44.409316	
325	0							
Gas	58.081640	5.107522	-.162870	.052985	-.003288	.010519	44.764060	
326	P0							
Gas	-4.606800	8.557584	.303882	-.056797	.004241	-.191215	62.588712	
327	S0							
Gas	-2.768323	8.625213	.265956	-.047287	.003543	-.225203	62.283064	
328	S10							
Gas	-24.704882	8.539369	.311713	-.059681	.004472	-.236467	59.650063	
329	T10-s,1							
Liquid	-113.004990	14.499996	.000002	-.000001			31.497276	
Solid	-133.763530	25.042523	-25.058750	18.219230	-3.514422	-1.202172	39.610356	

Constants for the Generation of Thermodynamic Properties (contd.)

			<u>1₇</u>	<u>1₁</u>	<u>1₂</u>	<u>1₃</u>	<u>1₄</u>	<u>1₅</u>	<u>1₆</u>
330	T1O								
Gas	11.894128	8.735039	.189703	-.030931	.002319	-.188863	65.784190		
331	ZrO								
Gas	20.454456	7.430978	-.289685	.062973	-.004609	.125174	66.622682		
332	O ₂								
Gas	-3.082757	8.021190	.546042	.007775	-.006116	-.216097	57.546610		
333	P0 ₂								
Gas	-78.565842	13.469032	.290861	-.065873	.004937	-.484903	74.376786		
334	S0 ₂								
Gas	-76.585312	13.005321	.740367	-.133370	.009961	-.552852	72.120604		
335	S10 ₂ -s,1								
Liquid	-210.675940	3.267316	20.334552	-7.141115	.301620	.137622	10.256793		
Solid	-227.020940	33.533141	-23.097580	11.313710	-1.739858	-2.588822	4.526772		
336	S10 ₂								
Gas	-79.783118	14.295497	.400278	-.090648	.0063802	-.5060F	69.262398		
337	T10 ₂ -s								
Solid	-222.514840	12.141150	13.350710	-10.196670	2.747208	-.055201	22.514830		
338	T10 ₂ -s,1								
Liquid	-217.984940	19.000000	-.000001	-.000004					
Solid	-231.977200	17.267437	1.126480	-.258052	.053745	-.378218	38.422816 30.420044		
339	T1O ₂								
Gas	-85.578202	14.471330	.284918	-.064614	.004855	-.457312	71.560022		
340	ZrO ₂ -s,1								
Liquid	-251.480960	20.000000	-.000002	.822937	-.064233	-.000001	37.634934		
Solid	-271.129840	22.398697	-.3.409967				34.735200		

Constants for the Generation of Thermodynamic Properties (Contd.)

		<u>17</u>	<u>11</u>	<u>12</u>	<u>13</u>	<u>14</u>	<u>15</u>	<u>16</u>
341	ZrO ₂							
Gas	-77.197966	14.574864	.217000	-.049198	.003591	-.421632	73.860208	
342	O ₃							
Gas	29.047072	11.965927	2.317604	-.984604	.134746	-.408850	68.810710	
343	SO ₃							
Gas	-103.477870	18.914115	1.809698	.193342	-.032500	-1.048307	78.506994	
344	Tl ₂ O ₃ -s,1							
Liquid	-345.393940	35.999998	-.000001					
Solid	-377.713060	36.209206	.131570	-.064203	.024098	-1.290489	.000001	69.535290
345	Tl ₃ O ₅ -s							56.080056
Solid	-597.877940	41.600030	8.000050	-.000070	-.000003	-	.000002	84.596724
346	P ₄ O ₆ -s							
Gas	-704.714580	51.083486	.382528	-.085641	.006318	-1.407032	199.582530	
347	P ₄ O ₁₀ -s							
Solid	-711.395020	5.331700	167.985000	-.34.561000	4.317000	.114540	.14.453590	
348	P ₄ O ₁₀							
Gas	-718.187420	75.030190	2.929403	-.662932	.049702	-4.338345	160.432750	
349	P-s							
Solid	-1.205590	3.837551	3.855380	-.261800	.051223	.036449	9.117028	
350	P-s,l							
Liquid	2.446148	6.292003	.000001	.000002				17.863191
Solid	2.225286	6.329999	.000010	.000020	.000002	-	.000001	17.312257
351	P							
Gas	77.64934	6.151183	-1.615799	.663240	-.061156	-.133362	46.243356	

Constants for the Generation of Thermodynamic Properties (Contd.)

		17	11	12	13	14	15	16
352	PS	19.647062	8.911469	.088725	-.004433	.000317	-.059191	66.481164
353	P ₂	39.556392	8.851769	.111965	-.013421	.001019	-.149131	62.022414
354	P ₄	23.605790	19.793835	.051772	-.011682	.000372	-.383980	88.755234
355	P ₄ S ₃ -s,1	49.196066	44.000020	.000020	.000010	-.000005	-.000003	102.757040
Liquid		-47.434844	34.999990	-.000050	-.000090	-.000008	-.000002	90.355682
356	P ₄ S ₃	-30.440002	36.999991	.000003				121.055720
357	S1-s,1	4.063520	-1.798016	14.971106	-8.476035	1.640271	1.326856	7.719378
Liquid		-1.218192	3.376136	6.884510	-.013890	.004226	.001183	9.915331
358	S ₁	65.418300	5.139423	-.221513	.121633	-.012464	.094618	46.819498
359	S ₁ S	13.823864	8.866381	.106888	-.011907	.000916	-.141241	63.392720
360	S ₂	27.752548	8.880099	.103814	-.008978	.000564	-.135211	64.521638
361	S ₁ S ₂ -s,1	38.730586	3.801890	22.291630	-5.935470	-.087052	.211745	20.787330
Liquid		-47.159994	12.899910	7.000070		.000016	.000004	29.516370

Constants for the Generation of Thermodynamic Properties (Contd.)

		<u>1₇</u>	<u>1₁</u>	<u>1₂</u>	<u>1₃</u>	<u>1₄</u>	<u>1₅</u>	<u>1₆</u>
362	S ₈	9.528309	43.621657	.065053	-.014739	.001101	-.598157	152.788940
363	S _{1-s,1}							
Liquid	10.266006	6.129998	.0000001					
Solid	-2.061463	5.613075	1.037119	-.328726	.035551	-.105974	18.628743	10.346968
364	S ₁							
Gas	109.125190	4.221513	.754595	-.144322	.009019	.132785	.45.664910	
365	S _{1₂}							
Gas	131.116120	12.439821	-1.510325	.274051	-.016484	-.722278	67.031025	
366	S _{1₃}							
Gas	140.814240	14.858244	.031350	-.007227	.000546	-.199297	77.530560	
367	T _{1-s,1}							
Liquid	1.493003	7.999998	.0000002	-.000001				
Solid	-1.451618	5.925830	2.060649	-.562132	.096616	-.051922	18.167172	14.128570
368	T ₁							
Gas	111.780990	4.467361	-.080391	.497023	-.054038	.199833	49.463762	
369	Z _{r-s,1}							
Liquid	476881	9.542918	-.709689	.163751	-.012419	-.584115	20.841346	
Solid	-2.130086	7.389096	.190688	.171876	-.019570	-.158490	17.882283	
370	Z _r							
Gas	145.200860	4.408072	1.422026	-.105337	.001491	.375265	49.912876	
371	LiBO _{2-s,1}							
Gas	-276.863280	54.825120	-18.435751	5.811510	-.610452	-7.032459	55.020628	

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Constants for the Generation of Thermodynamic Properties (Contd.)

		<u>1.7</u>	<u>1.1</u>	<u>1.2</u>	<u>1.3</u>	<u>1.4</u>	<u>1.5</u>	<u>1.6</u>
373	<chem>CCl2F2</chem>							
Gas	-10.740963	24.985195	.559021	-.126692	.009509	-.989307	96.945708	
374	<chem>TiF</chem>							
Gas	-59.101938	8.869543	.126917	-.010974	.000820	-.140340	65.880238	
375	<chem>LiNaO</chem>							
Gas	-71.421216	13.557494	.233400	-.053092	.003998	-.150605	75.425440	
376	<chem>Li2TiO3-s,1</chem>							
Gas	-336.446600	-23.870384	98.040270	-43.809380	6.353690	4.359097	8.020211	
378	<chem>MgTi2O3-s,1</chem>							
Gas	-565.140260	-13.936244	82.819040	-28.231695	3.102851	5.383975	25.628946	
379	<chem>Mg2TiO4-s,1</chem>							
Gas	-479.536400	-27.327780	93.405550	-32.280402	3.592968	6.430622	3.332577	
380	<chem>NaO4-s,1</chem>							
Gas	-3.591929	22.716120	46.074100	-23.057100	.019060	.002010	64.717342	

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